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ECBC-TR-102

**COMPARISON OF PORTABLE RAMAN INSTRUMENTS
FOR USE IN THE SINGLE CAIS ACCESS AND
NEUTRALIZATION (SCANS) PROJECT**

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PREFACE

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CONTENTS

1. INTRODUCTION	7
2. BACKGROUND	7
3. CAIS MATERIAL.....	8
3.1 Description.....	8
3.2 Samples.....	9
4. RAMAN INSTRUMENT COMPARISON	9
4.1 Specifications.....	9
4.2 Calibration	9
4.3 Fiber Optic Probe Performance	11
5. RAMAN SPECTRA COMPARISON.....	12
5.1 Spectral Data.....	12
5.2 Spectral Range	12
5.3 Spectral Resolution.....	14
5.4 White Light Correction.....	14
5.5 Computer Hardware and Software	15
6. CONCLUSIONS	15
LITERATURE CITED	17
APPENDIX A: Spectra Obtained with the INEEL Raman System.	19
APPENDIX B: Spectra Obtained with the InPhotote Raman System.....	35
APPENDIX C: Spectra Obtained with the Sentinel Raman System.	43
APPENDIX D: Spectra Obtained with the RS2000 Raman System.	51

FIGURES

1: Cyanogen chloride spectrum using the INEEL System with the Chromex probe and the EIC probe	12
2: Resolution Test - Lewisite in Chloroform	14

TABLES

1: Contents of CAIS.....	8
2: Samples Tested.....	9
3: Raman Instruments Specifications	10
4: Summary of Raman analysis of CAIS standards and recovered CAIS material	13
5: Main Raman peak positions for CAIS chemicals.....	13
6: SCANS Requirements Checklist	16

COMPARISON OF PORTABLE RAMAN INSTRUMENTS FOR USE IN THE SINGLE CAIS ACCESS AND NEUTRALIZATION (SCANS) PROJECT

1. INTRODUCTION

The U.S. Army's Product Manager for Non-stockpile Chemical Material (PMNSCM) currently uses Raman instruments to identify the contents of Chemical Agent Identification Sets (CAIS) in two fielded systems; the Rapid Response System (RRS) and the Mobile Munitions Assessment System (MMAS). PMNSCM is now looking at Raman instruments to meet the needs of a new project; the Single CAIS Access and Neutralization System (SCANS). SCANS will consist of a man-portable Raman spectroscopy system for CAIS characterization, a self-contained system for the destruction and neutralization of the CAIS items, and a packaging process for final disposal of the waste.

This report details the comparison of four different Raman systems and assesses their ability to meet the needs of the SCANS program. In this analysis we looked at Raman systems that have already been developed for the RRS (EIC RS2000) and the MMAS (Idaho National Engineering and Environmental Laboratory packaged Chromex spectrometer). We also tested two new commercially available Raman instruments manufactured by InPhotonics (a subsidiary of EIC) and Chromex. InPhotonics and Chromex brought their instruments (the InPhotote and Sentinel, respectively) to the Edgewood Chemical Biological Center (ECBC) for testing with CAIS standards and actual recovered CAIS material. Our objective in these tests was to determine whether the new instruments from InPhotonics and Chromex met the sensitivity, spectral coverage, and resolution requirements for identifying CAIS material. We also wanted to compare their performances to the fielded instruments. The new instruments are smaller, easier to calibrate, and we expect cheaper than the current systems. Either would be preferred for the SCANS mission if it were found to meet the criteria described above.

Raman spectra of the CAIS material and standards had previously been obtained for the RRS Raman^{1,2} instrument and the Idaho National Engineering and Environmental Laboratory (INEEL) instrument. No additional testing was needed for the RS2000. The INEEL instrument, however, was brought to ECBC for additional testing using two new fiber optic probes. The INEEL system originally used a fiber bundle probe that proved to be unnecessarily large and susceptible to breakage. The new probes, like the probes used in the other instruments tested, use a single excitation and emission fiber.

2. BACKGROUND

Between 1920 and 1960 more than 110,000 CAIS were produced to train personnel in the identification of chemical agents. These chemical agents and industrial chemicals were stored in glass ampoules and bottles. These ampoules and bottles were packaged in boxes or metal shipping containers. Many of the sets were expended during training, however, unused CAIS were buried in land fills and stored in bunkers. This method of disposal was the accepted practice at the time. About 20 percent of these left over CAIS were destroyed in the late 70's and early 80's. It is expected that both complete and partial CAIS consisting of loose bottles and ampoules will be discovered and recovered from various burial grounds.

The Rapid Response System analyzes CAIS using a Raman spectrometer (EIC RS2000). The RRS will be deployed at sites where CAIS material is currently located in large quantities. Its Raman spectrometer analysis system is mounted in a conventional instrument cabinet with shock isolation mounts housed in the Operations Trailer. The ampoules and bottles are interrogated with a fiber optic probe inside a glove box in the Operations Trailer.

3. CAIS MATERIAL

3.1 Description

Several different kinds of chemical agent identification sets were developed and fielded. Liquid samples in the sets were sealed in glass ampoules or 4 ounce bottles, and the solid samples were stored only in glass bottles. Two ampoule sizes were used; 1.875 inches in diameter by approximately 4.625 inches long and 1 inch diameter by 7.5 inches long. The contents of the bottles were typically etched in the glass and remained legible. When initially prepared, the contents of the liquid items in the CAIS were either colorless or had a slight yellow tint. Over the years of storage, however, many of the items have degraded and are now highly colored. Unfortunately, the color is not necessarily indicative of the contents. Based on the analyses of recovered CAIS items, the contents of an ampoule containing a clear liquid could be anyone of 4 different chemicals or mixtures. Recovered CAIS items containing lewisite in chloroform have ranged in color from clear to brown. Items containing mustard in chloroform have been either clear or dark red to black. Some phosgene samples have also been red. Table 1 lists the contents of the CAIS.

Table 1: Contents of CAIS.

STORED IN AMPOULES
5% sulfur mustard in chloroform
5% lewisite in chloroform
10% nitrogen mustard in chloroform
neat phosgene
neat cyanogen chloride
50% chloropicrin in chloroform
GA simulant
STORED IN BOTTLES
neat sulfur mustard
sulfur mustard adsorbed on charcoal
lewisite adsorbed on charcoal
nitrogen mustard (HN-1 or HN-3) adsorbed on charcoal
chloropicrin adsorbed on charcoal
solid chloroacetophenone
solid triphosgene (CG simulant)
sold adamsite

3.2 Samples

Table 2 lists the samples actually used for the comparison tests. The CAIS standards containing chemical warfare agents were prepared from spectrophotometric grade chloroform (Fisher) and chemical agent standards analytical reference material (CASARM) grade distilled mustard (HD), lewisite (L), and nitrogen mustard (HN-1 and HN-3). Chloropicrin and chloroacetophenone were purchased from Kodak and Aldrich, respectively. The adamsite and cyanogen chloride were of unknown origin.

The CAIS items listed are actual recovered CAIS materials that have been analyzed by GC/MS. Because of this analysis, these items have been removed from their original ampoules, and are now stored in glass bottles. The Raman spectra were obtained from the samples in these glass bottles.

Table 2: Samples Tested

	DESCRIPTION
STANDARDS	Adamsite (DM) Solid Chloroacetophenone (CN) Solid Chloroform/Chloropicrin (50/50) HD (5%) in Chloroform HD adsorbed onto charcoal HD (neat) HN-1 adsorbed onto charcoal HN-1 Nitrogen Mustard HN-3 Nitrogen Mustard Lewisite (5%) in Chloroform Lewisite (neat)
CAIS ITEMS	CAIS item OG0101: PS (41.14%) in Chloroform CAIS item OG0105: L (2.7%) in Chloroform CAIS item OG0207: H (2.82%) in Chloroform CAIS item OG0406: L (2.56%) in Chloroform CAIS item PO1305: Phosgene (CG) CAIS item PO1307: L (9.37%) in Chloroform

4. RAMAN INSTRUMENT COMPARISON

4.1 Specifications

The characteristics of the four Raman instruments tested are detailed in Table 3. The INEEL system, Sentinel, and EIC RS200 run off of standard 110V-AC. InPhotonics advertises that the InPhotote can operate off of 110V-AC, 12V-DC, or portable battery pack.

4.2 Calibration

Like the RRS Raman system, personnel with little knowledge of or experience with Raman spectroscopy will operate the SCANS. Because of this, the Raman system for SCANS will rely on spectral identification software (Spectral ID™ by Galactic Industries) to identify the suspect CAIS contents. These spectral identification routines

require that the measured spectral lines not deviate from the values stored in the spectral library by more than 2 or 3 wavenumbers. Laser wavelength shifts and/or slight optical misalignments in the spectrometer can result in spectral shifts of more than a few wavenumbers (cm^{-1}). For this reason, the SCANS Raman instrument needs to possess software capable of adjusting for these small spectral shifts. The software will also alert the operator to more serious misalignment problems that would require adjustment by the manufacturer. As a further precaution, during actual field analyses the operator will transmit the spectra through a phone modem to a senior scientist at ECBC familiar with Raman spectroscopy and CAIS fills to confirm interpretation of the spectral data and identification of the CAIS fill prior to treatment

Table 3: Raman Instruments Specifications

	<i>InPhotonics Inphotote</i>	<i>Chromex Sentinel</i>	<i>INEEL Chromex</i>	<i>EIC RS2000</i>
Spectrometer				
Dimensions (in)				
Height	9	8	18½	8
Width	10	15	27¼	16
Length	16	18	34¼	26
Weight (lbs)	20	25	<150	50
Resolution (cm^{-1})	~6	~6	7	2
Wavenumber Range (cm^{-1})	234 to 2590	300 to 1850 ^a	117 to 3300 ^b	720 to 3092
Calibration Procedure	On demand (automatic)	Continuous, automatic	On demand (automatic)	Not automatic
Laser				
Dimensions (inches)	Included in Spectrometer	Included in Spectrometer	Included in Spectrometer	10" x 3½" x 5½"
Wavelength (nm)	785	~810	785	785
Power (mW)	300	115	300	300
Other Instrumentation	None	None	None	CCD Controller 13¼" x 6¾" x 8"
Fiber Optic Probe				
Size	0.5" diam, 4" length	8" x 3" x 2.5"	8" x 3" x 2.5" ^c	0.5" diam, 4" length
Fiber Cable Type	1 excitation & 1 collection	1 excitation & 1 collection	1 excitation & 1 collection	1 excitation & 1 collection
Exc. Fiber Diam. (μm)	90	50	50	90
Emiss. Fiber Diam. (μm)	200	600	600	200
Focal Length (mm)	10	50	50	10
Cable Length Tested	25	4	25	25

Notes

- a. Sentinel Range Upgradable to 2900 cm^{-1}
- b. Due to movement of the detector, the actual range for the test was -873 to 2771 cm^{-1}
- c. The INEEL system was tested with both probe designs

The Sentinel has the most sophisticated spectral calibration procedure of the four instruments tested. Using what Chromex calls the "Sure_Cal" system it monitors the laser wavelength as well as the spectral lines of an internal calibration source providing both frequency and intensity calibration. Because the laser line is monitored in real time, Chromex can use a less stable and longer lived laser than is used by the other instruments. The Sentinel was designed for use in process monitoring where it would be required to run continuously and unattended. For that application, the Sentinel is clearly the best choice.

The EIC RS2000 system has no set calibration procedure. Because the spectral coverage includes the laser line, any drift in the laser can be observed in the spectra. If the laser wavelength has drifted, the operator can calculate the offset and adjust the laser wavelength using software provided.

The INEEL system and the InPhotote can calibrate on demand using software provided. In each case, the program compares the spectrum of a standard sample such as tylenol with a previously stored standard spectrum. After comparing the peak positions, the program will automatically adjust the spectral axis (cm^{-1}) to match the stored spectrum. The InPhotote can even use the spectral lines from the computer screen for calibration. The calibration procedures provided in the INEEL system and InPhotote should be adequate for the SCANS mission where the instrument would be used at most for a few hours at a time.

4.3 Fiber Optic Probe Performance

The EIC RS2000 and InPhotote used the EIC fiber optic probe. The Sentinel used the Chromex probe, and the INEEL system was tested with both probe designs. The probe specifications are provided in Table 3. Both probes performed well in the tests. In the tests with both probes using the INEEL system, the spectra obtained with the EIC probe had a higher background from the glass bottles and vials. This was not observed with the EIC probe used with either the InPhotote or EIC RS2000 spectrometers. Improper positioning of the probe with respect to the sample may have caused the increased background.

From the data obtained in the tests, neither probe has a clear advantage in performance. The EIC probe is smaller and is compatible with the RRS instrument and the INEEL system developed for MMAS. Because the Sentinel uses a different excitation wavelength (~810 nm vs. 785 nm), it cannot use the EIC probes. Another issue with the Chromex fiber optic probe is the transmission loss observed in the 2050 to 2300 cm^{-1} region in the INEEL system tests. Chromex has determined that this is due to poor quality optical fiber used in making that probe. Chromex may not have observed this problem using the shorter (4-meter) fiber lengths in previous evaluations of system performance. Since the transmission loss increases exponentially with fiber length, however, the problem was very evident with the 25-meter fiber optic cable used in the tests. In the tests at ECBC, this transmission loss prevented us from observing a characteristic peak from cyanogen chloride (Figure 1). Chromex has agreed to replace the INEEL probe with a new Chromex probe that does not have this problem. The Sentinel tests using the same kind of probe did not demonstrate this problem because the instrument tested only covered the spectral range to 1850 cm^{-1} .

5. RAMAN SPECTRA COMPARISON

5.1 Spectral Data

The Raman spectra obtained in the instrument tests are collected in the appendices as follows: Appendix A - INEEL system, Appendix B - InPhotote, Appendix C - Sentinel, Appendix D - EIC RS2000. Table 4 summarizes the results of the data collection in terms of each instrument's ability to identify the contents of CAIS standards and recovered CAIS material. We obtained spectra of tear gas (CS) with the InPhotote system, but since we only measured it with the one instrument CS was not included in the comparison. We also had measured different recovered CAIS material with the RS2000 than was used in the tests with the other instruments.

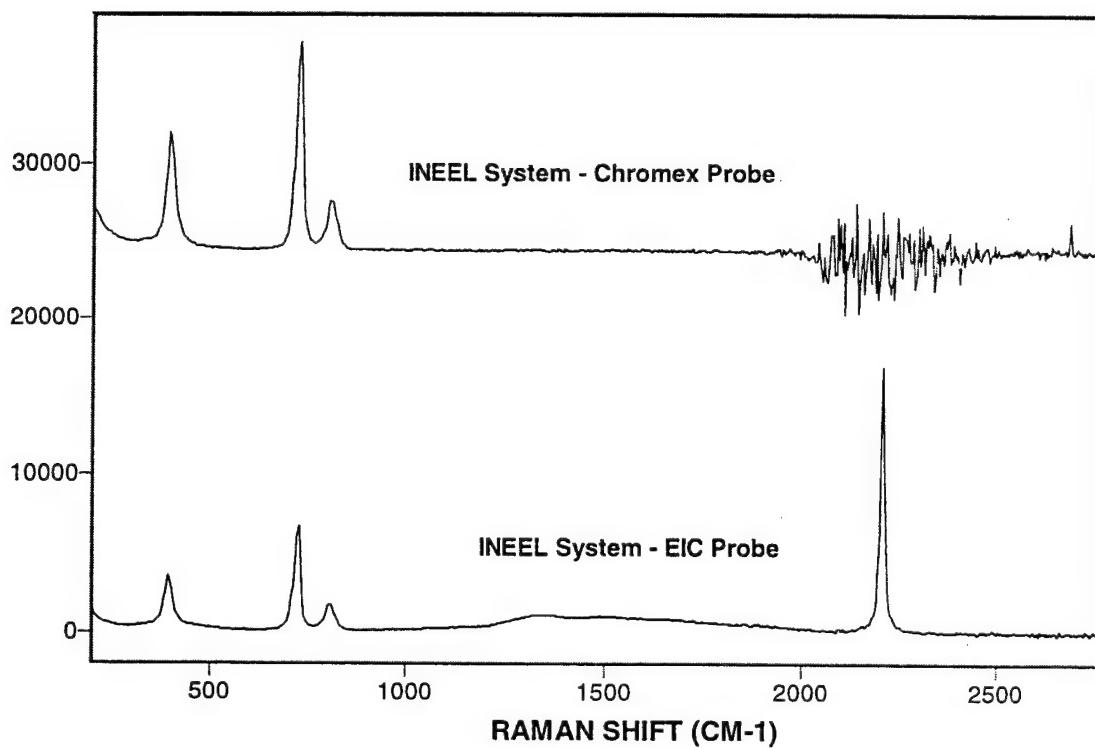


Figure 1: Cyanogen chloride spectrum using the INEEL system with the Chromex probe and the EIC probe.

5.2 Spectral Range

The characteristic Raman bands used for identifying CAIS material are listed in Table 5. This table was generated using the EIC RS2000, which has a spectral range covering the entire Raman spectrum up to 3092 cm^{-1} . Although a spectral identification does not require the collection of the entire Raman spectrum, it was determined that any new instrument should cover at least the spectral region from 340 to 2300 cm^{-1} . This region contains most of the relevant spectral lines and includes the CN stretching region around 2200 cm^{-1} , which is diagnostic for cyanogen chloride. With the exception of the

Sentinel, all of the instruments tested met this requirement. The Sentinel does offer an optional configuration with a spectral range of 2900 cm⁻¹.

Table 1: Summary of Raman analysis of CAIS standards and recovered CAIS material

Source	Material Analyzed	INEEL - Chromex Probe	INEEL - InPhotonics Probe	Inphotote	Sentinel	EIC RS2000 (RRS)
CASARM	Adamsite solid	Y	Y	Y	Y	Y
	Chloroacetophene solid	N	Y	Y	Y	Y
	Distilled sulfur mustard/chloroform	Y	Y	Y	Y	Y
	Distilled sulfur mustard neat	Y	Y	Y	Y	Y
	Nitrogen mustard on charcoal	N	N	N	NR	N
	Nitrogen mustard (HN-1)	Y	Y	Y	Y	NR
	Nitrogen mustard (HN-3)	N	N	N	N	NR
	Cyanogen chloride	Y*	Y	NR	NR	Y
	Lewisite/chloroform	Y	Y	Y	Y	Y
	Lewisite neat	Y	Y	Y	Y	NR
RECOVERED CAIS	Chloropicrin/chloroform	Y	Y	Y	Y	Y
	Lewisite/chloroform	P	P	P	P	P
	Distilled sulfur mustard/chloroform	P	P	P	P	P
	Chloropicrin/chloroform	Y	Y	Y	Y	Y
* The large peak at 2207 cm ⁻¹ was not observed, but identification was possible using other peaks.						
Y - Readable						
N - Not Readable						
NR - Not Run						
P - Partial (Chloroform Only)						

Table 2: Main Raman peak positions for CAIS chemicals.

AGENT	PEAK POSITIONS (cm ⁻¹)				
	1	2	3	4	5
CG	302	444	571	836	1809
Chloroform	261	367	668		
CK	391	726	2207		
CN	1000	1596	1693		
DM	847	884	1215	1272	1309
GA Simulant	214	855	1298	1451	1736
HD	704	1295	1426		
HN-1	1450	2961			
L	395	1290	1554		
PS	296	440	708	842	1309

5.3 Spectral Resolution

The requirement for spectral resolution is that the system be capable of resolving the lewisite and chloroform peaks at 395 cm^{-1} and 367 cm^{-1} , respectively. All of the instruments tested were able to resolve those peaks, and thus, identify lewisite in chloroform. Figure 2 shows spectra of this region obtained with each of the instruments. The EIC RS2000 has the highest resolution and provided the best separation between the chloroform and lewisite peaks. The InPhotote and Sentinel have comparable resolutions and their abilities to separate these lines are very similar.

The INEEL system had the poorest resolution, but it is still able to distinguish the lewisite band from the chloroform band. The INEEL has adjustable slits that can be narrowed to improve the resolution while sacrificing some sensitivity. The other instruments do not use an entrance slit, and for them, the emission fiber diameter defines the entrance aperture. The INEEL instrument also comes equipped with 2 other gratings that can provide higher resolution with a reduced spectral range. The spectral range and resolution for these gratings using a $50 \mu\text{m}$ slit are $1800/4 \text{ cm}^{-1}$ and $950/2 \text{ cm}^{-1}$.

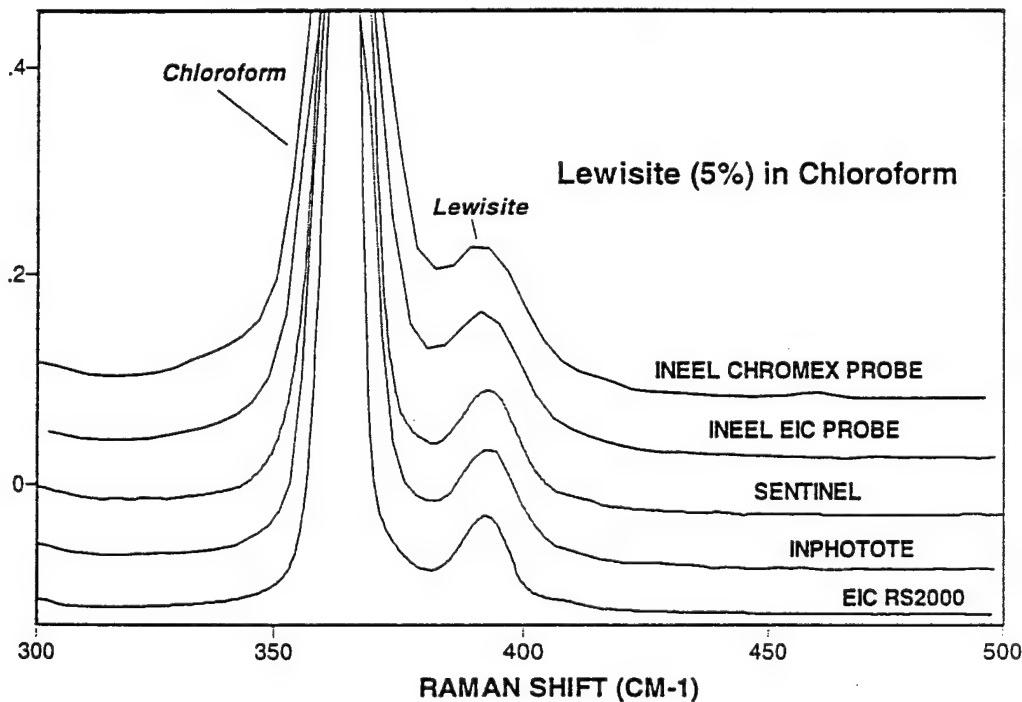


Figure 2: Resolution Test - Lewisite in Chloroform

5.4 White Light Correction

The Raman system (spectrometer, fiber-optic probe, and CCD detector) has its own "spectrum"; that is, its spectral response is not flat over the entire spectral region. The Sentinel accounts for this variation using built in calibration lines. The EIC RS2000 and the InPhotote require that a calibration spectrum be measured using a flashlight as a white light source. Since the flashlight's output is nearly the same for all wavelengths

(wavenumbers) in the region covered by the Raman system, the spectrum obtained with the flashlight is simply the Raman system's response function or spectrum. This spectrum should only have to be measured once, assuming the fiber optic probe is not changed. Software in the RS2000 and InPhotote automatically divides the spectrum collected by this white light spectrum.

The Chromex spectrometer used in the INEEL instrument does not automatically perform a white light correction. During the test, a spectrum of a diffused flashlight beam was measured, and the corrections were performed offline with software provided by Chromex. In spectra where the Raman signal is large, the correction does not significantly alter the spectrum.

5.5 Computer Hardware and Software

A laptop computer controls the InPhotote and Sentinel. The InPhotote connects via a PCMCIA card while the Sentinel uses a standard serial port. The INEEL system and the EIC RS2000 both require a computer capable of accommodating a full size card. The INEEL system is currently using a Dolch FieldPAK™ computer, while the EIC RS2000 in the RRS uses a desktop computer. The EIC RS2000 can operate with the FieldPAK™ computer also.

Each instrument company provides its own data collection software. The INEEL system and Sentinel (both manufactured by Chromex) use the same software, while the RS2000 and InPhotote (both manufactured by EIC or its subsidiary InPhotonics) use the EIC data collection software. All of the systems, however, use Galactic Industries Grams/32™ software for data display and manipulation.

6. CONCLUSIONS

All of the instruments tested are capable of identifying the contents of CAIS items within the limits of the capabilities of Raman spectroscopy in general. None of the instruments are able to detect HD or HN-1 on charcoal, nor can they positively identify some of the HD and L in chloroform samples that possess large fluorescence backgrounds.

A summary of the instrument evaluations is provided in Table 6. This table provides a qualitative assessment on the instruments' abilities to meet the SCANS requirements for sensitivity, resolution, spectral coverage, size and weight, and calibration. The EIC RS2000 does not meet the size or calibration requirement. The RS2000 is larger than the Chromex instrument used in the INEEL system, which was determined to be the largest system acceptable for the SCANS mission. It also has no automatic calibration procedure, although this could possibly be remedied by a software modification. The EIC RS2000 that was first purchased for the RRS still has the best combination of resolution and spectral range of any of the instruments tested and probably of any "portable" instrument on the market.

The Sentinel is really an improved (for process monitoring applications) version of the Chromex instrument packaged by INEEL, and it would require repackaging similar to the current INEEL system. The Sentinel has the most complete and automatic instrument calibration procedure of any of the instruments tested. This feature is extremely important in applications where continuous and unattended operation is

required, but not as critical for the SCANS mission where the instrument is expected to be used briefly and intermittently. The calibration procedures used by the InPhotote and INEEL system should be adequate for the SCANS project.

The InPhotote is the smallest of the instruments tested and could be carried onto a commercial airline. The manufacturer does, however, suggest that the InPhotote be placed in an additional protective case if it is shipped or sent as standard luggage. Because it uses the same laser wavelength as the INEEL system and the RRS instrument, the InPhotote can use the same fiber optic probes. This ability to share probes may be useful in the event one or more of the SCANS probes become damaged.

Table 6: SCANS Requirements Checklist

	InPhotonics InPhotote	Chromex Sentinel	EIC RS2000	Chromex Raman 2000
Sensitivity	✓	✓	✓	✓
Resolution	✓	✓	✓+	✓
Spectral Coverage	✓	✓	✓+	✓
Size and Weight	✓+	✓	✓-	✓
Calibration	✓	✓+	✓-	✓

✓ Meets SCANS requirements
 ✓+ Surpasses SCANS requirements
 ✓- Does not meet SCANS requirements

LITERATURE CITED

1. Chatfield, Mark D.; Carrabba, Michael M.; Haas, John W.; MacIver, Brian K.; and Christesen, Steven D.; *Evaluation of Fiber Optic Raman Spectroscopy Systems for the Non-Intrusive Segregation of Chemical Agent Identification Sets*, ERDEC-CR-178, U.S. Army Edgewood Research, Development and Engineering Center, Aberdeen Proving Ground, MD, May 1995.
2. Christesen, Steven; MacIver, Brian; Procell, Lawrence; Sorrick, David; Carrabba, Michael; and Bello, Job; "Nonintrusive Analysis of Chemical Agent Identification Sets Using a Portable Fiber-Optic Raman Spectrometer," *Applied Spectroscopy*, 53(7), pp 850-855 (1999).

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APPENDIX A: Spectra Obtained with the INEEL Raman System.

FIGURES

A- 1: Adamsite (DM) - Chromex Probe.....	20
A- 2: Adamsite (DM) - InPhotonics Probe	20
A- 3: Chloroacetophenone (CN) - Chromex Probe.....	21
A- 4: Chloroacetophenone (CN) - InPhotonics Probe	21
A- 5: 50% Chloropicrin (PS) in Chloroform - Chromex Probe	22
A- 6: 50% Chloropicrin (PS) in Chloroform - InPhotonics Probe.....	22
A- 7: HD (neat) - Chromex Probe.....	23
A- 8: HD (neat) - InPhotonics Probe.....	23
A- 9: 5% HD in Chloroform - Chromex Probe.....	24
A- 10: 5% HD in Chloroform - InPhotonics Probe.....	24
A- 11: Nitrogen Mustard (HN-1) - Chromex Probe.....	25
A- 12: Nitrogen Mustard (HN-1) - InPhotonics Probe	25
A- 13: Lewisite (neat) - Chromex Probe.....	26
A- 14: Lewisite (neat) - InPhotonics Probe.....	26
A- 15: 5% Lewisite in Chloroform - Chromex Probe	27
A- 16: 5% Lewisite in Chloroform - InPhotonics Probe.....	27
A- 17: Cyanogen Chloride - Chromex Probe.....	28
A- 18: Cyanogen Chloride - InPhotonics Probe.....	28
A- 19: CAIS Item OG0105 - Chromex Probe.....	29
A- 20: CAIS OG0105 - InPhotonics Probe	29
A- 21: CAIS OG0101 - Chromex Probe	30
A- 22: CAIS OG0101 - InPhotonics Probe	30
A- 23: CAIS OG0207 - Chromex Probe	31
A- 24: CAIS OG0207 - InPhotonics Probe	31
A- 25: CAIS OG0406 - Chromex Probe	32
A- 26: CAIS OG0406 - InPhotonics Probe	32
A- 27: CAIS PO1305 - Chromex Probe	33
A- 28: CAIS PO1305 - InPhotonics Probe	33
A- 29: CAIS PO1307 - Chromex Probe.....	34
A- 30: CAIS PO1307 - InPhotonics Probe.....	34

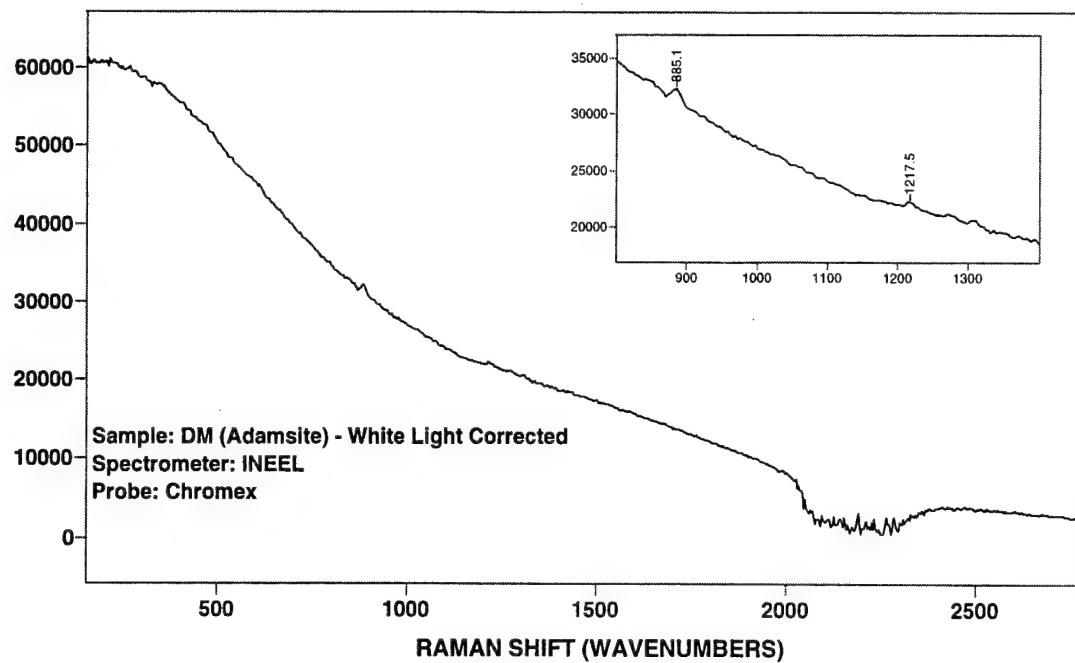


Figure A- 1: Adamsite (DM) - Chromex Probe

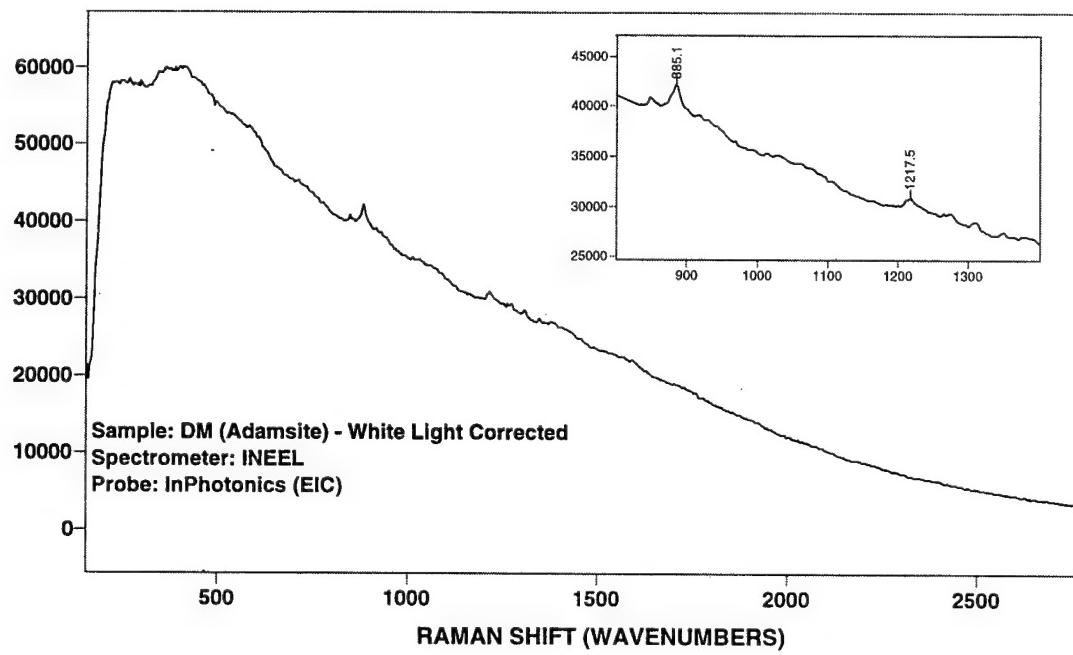


Figure A- 2: Adamsite (DM) - InPhotonics Probe

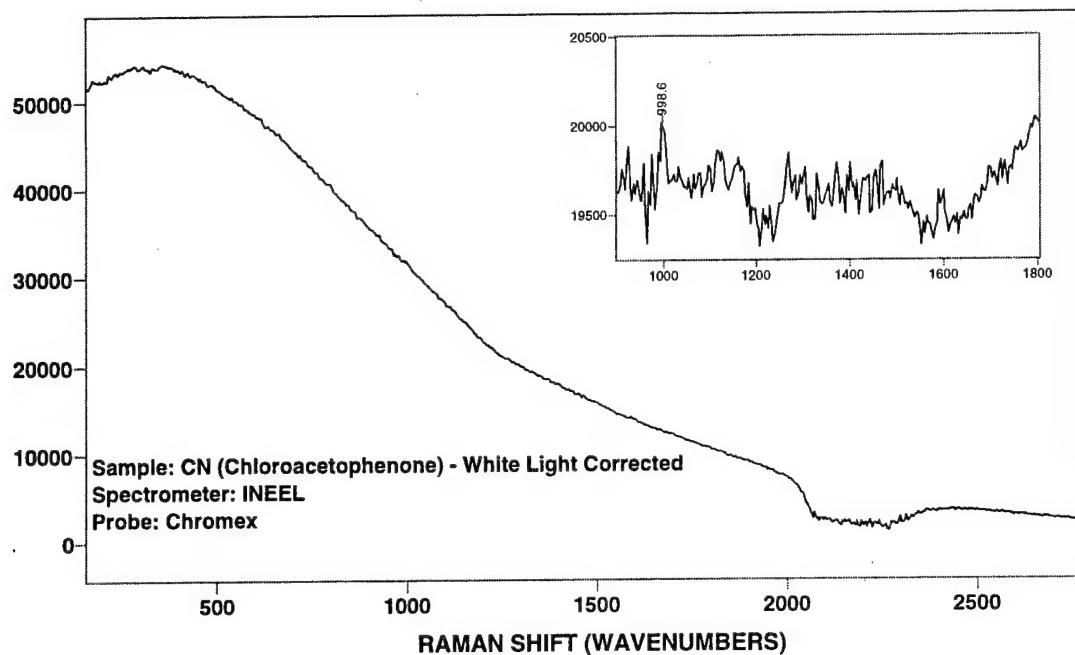


Figure A- 3: Chloroacetophenone (CN) - Chromex Probe

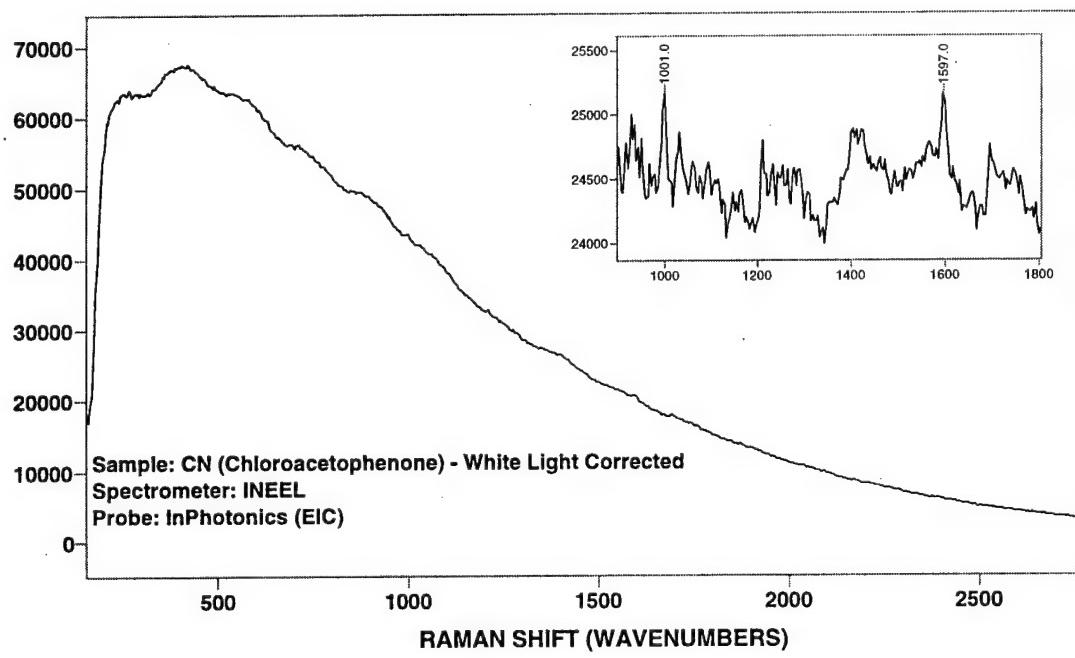


Figure A- 4: Chloroacetophenone (CN) - InPhotonics Probe

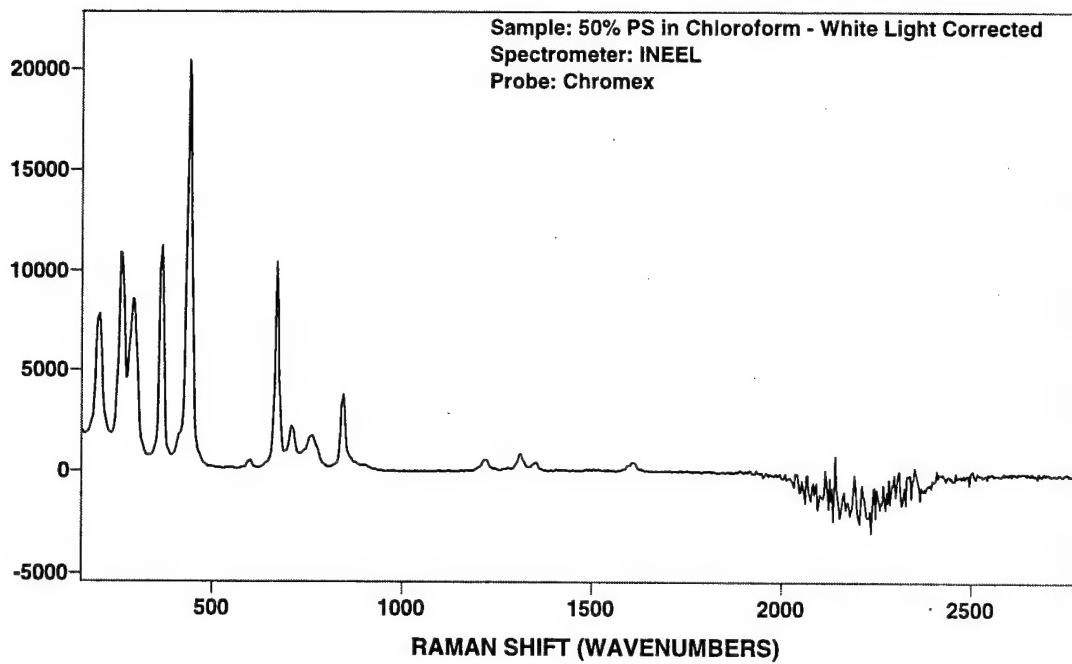


Figure A- 5: 50% Chloropicrin (PS) in Chloroform - Chromex Probe

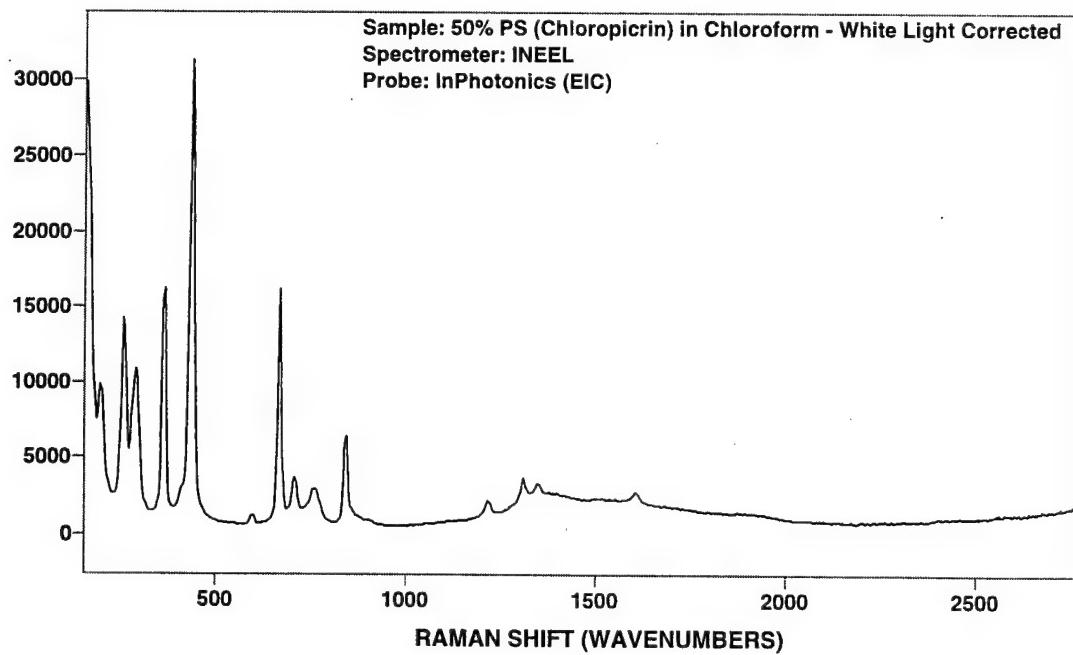


Figure A- 6: 50% Chloropicrin (PS) in Chloroform - InPhotonics Probe

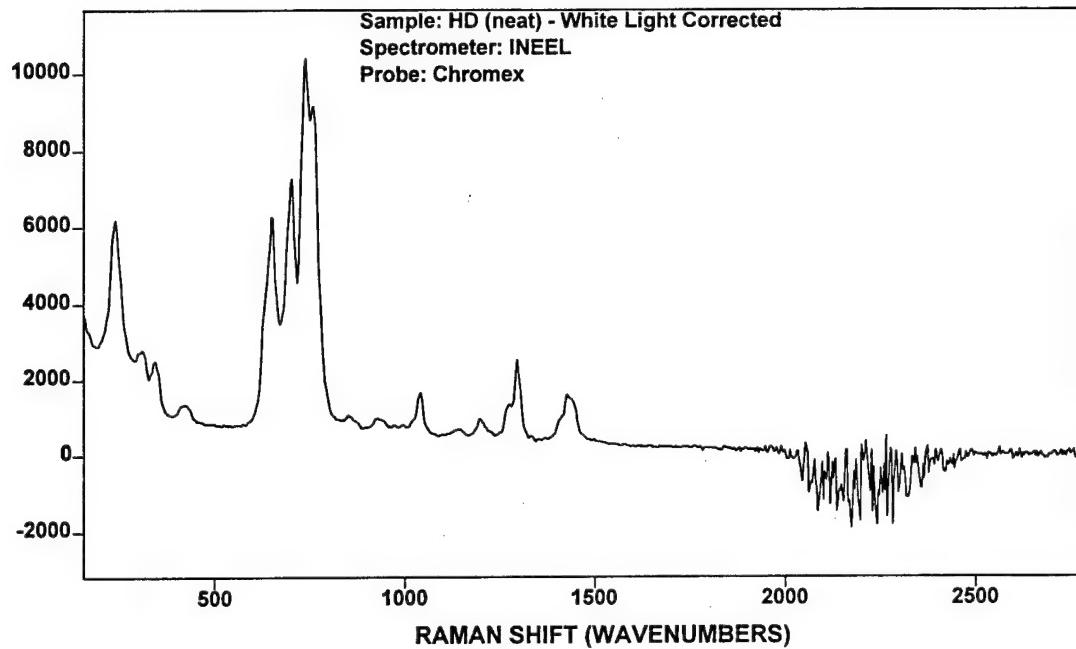


Figure A- 7: HD (neat) - Chromex Probe

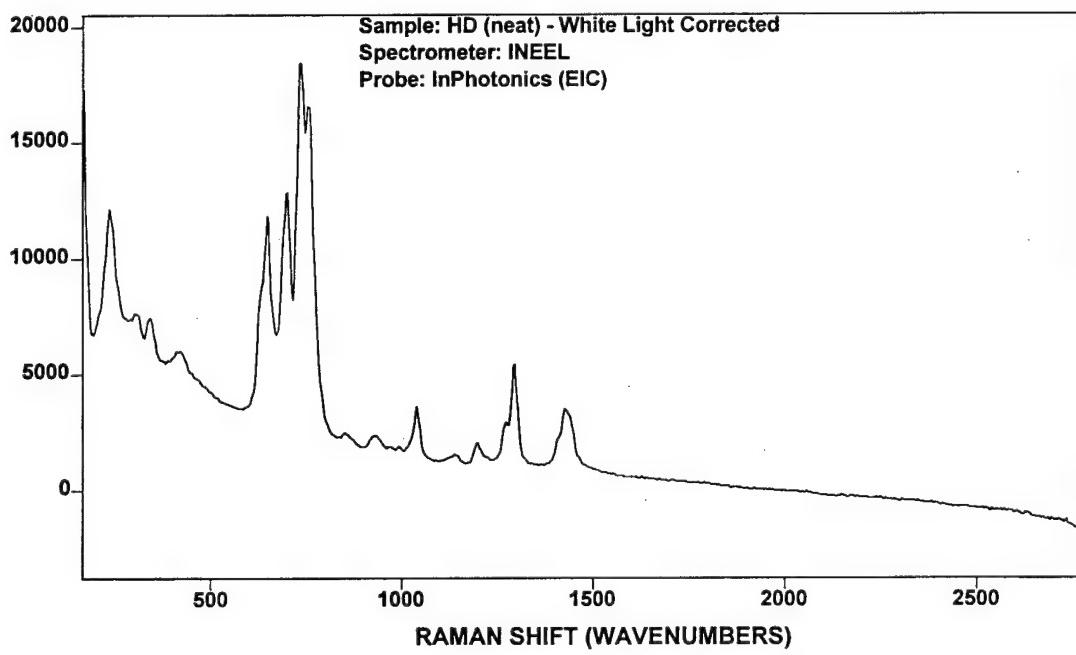


Figure A- 8: HD (neat) - InPhotonics Probe

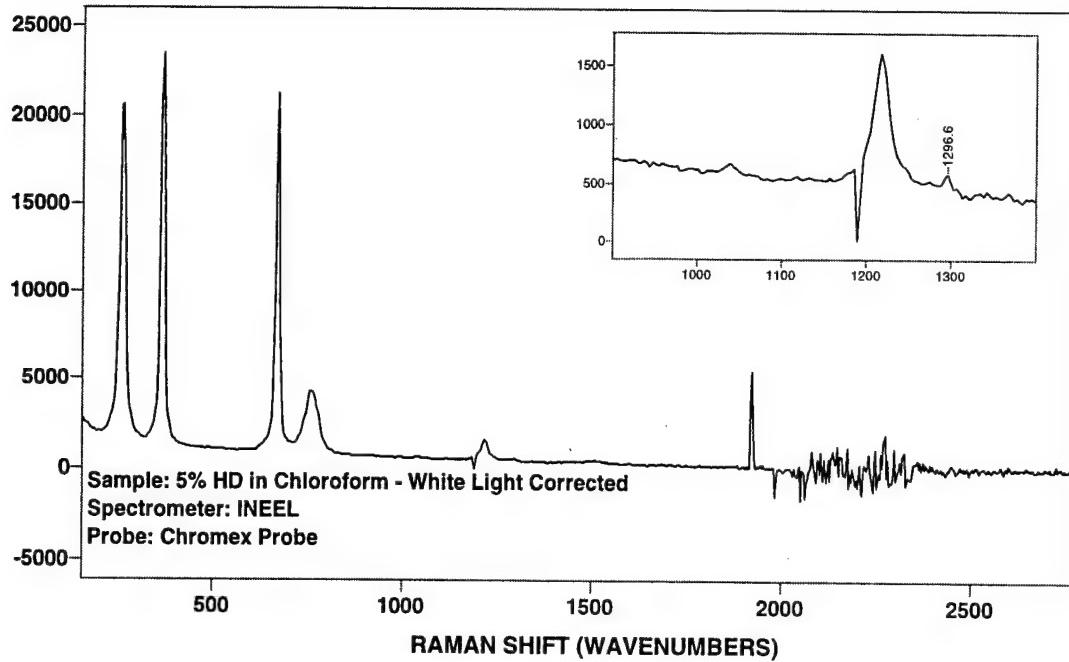


Figure A- 9: 5% HD in Chloroform - Chromex Probe

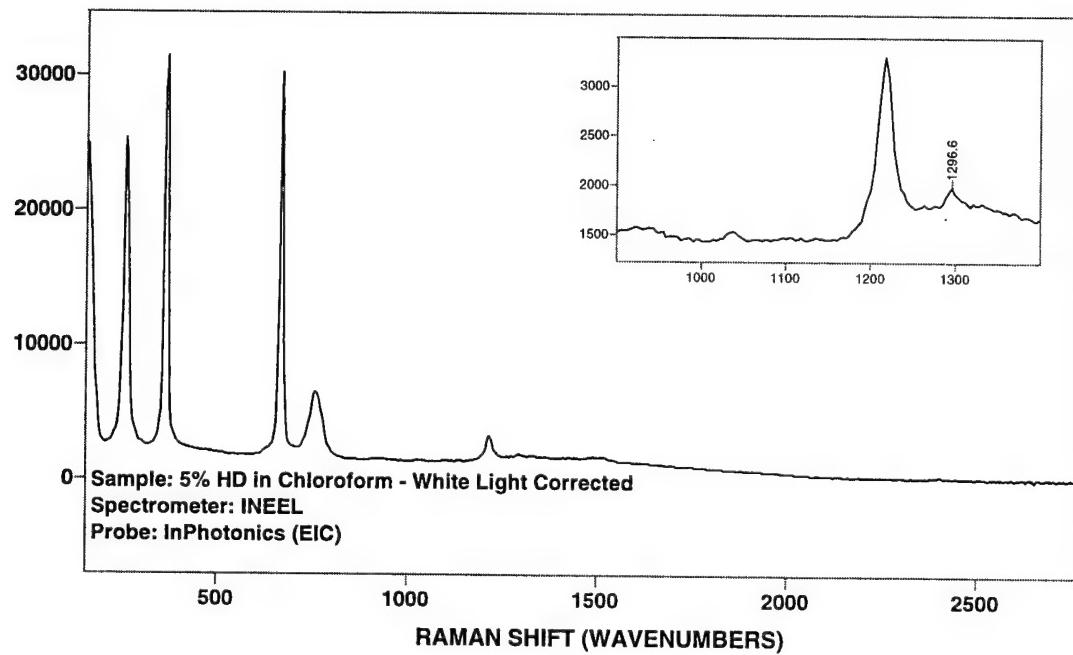


Figure A- 10: 5% HD in Chloroform - InPhotonics Probe

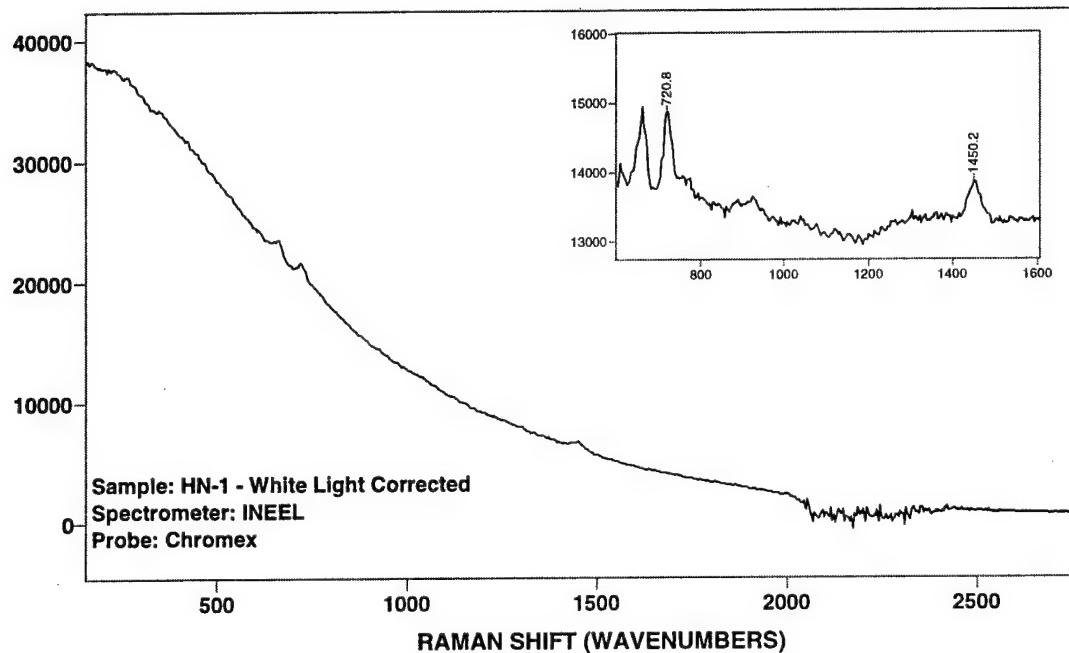


Figure A- 11: Nitrogen Mustard (HN-1) - Chromex Probe

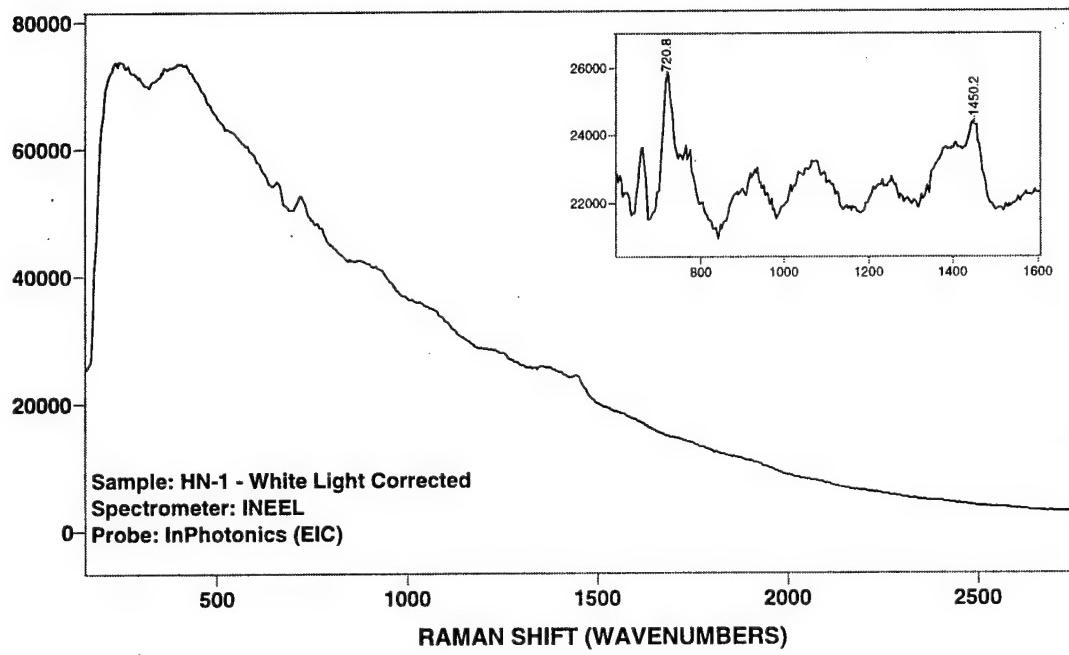


Figure A- 12: Nitrogen Mustard (HN-1) - InPhotonics Probe

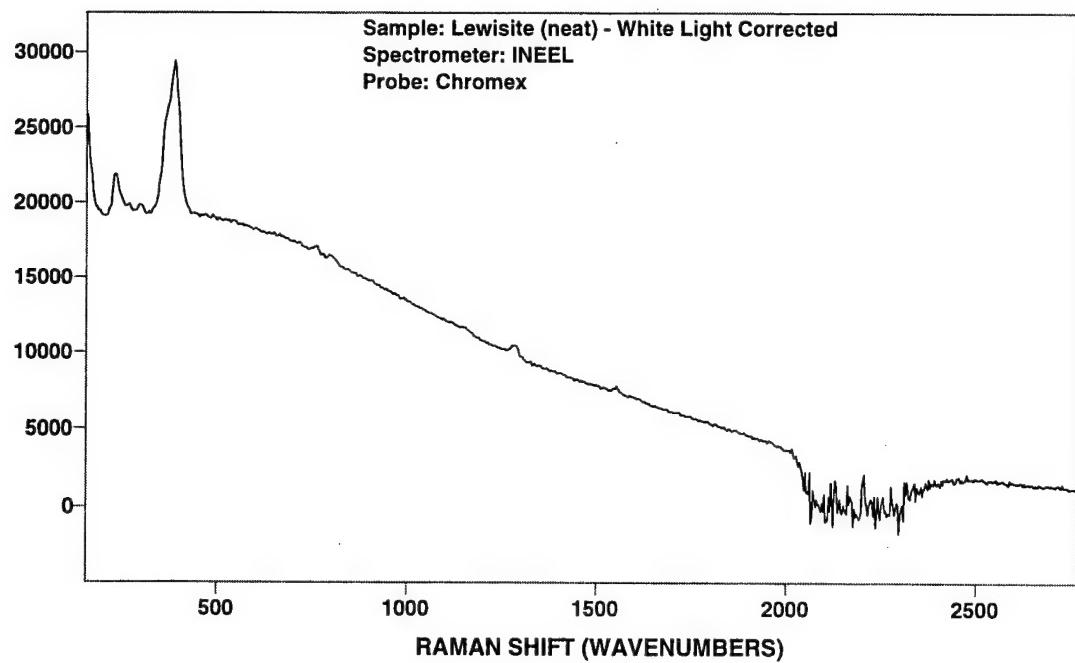


Figure A- 13: Lewisite (neat) - Chromex Probe

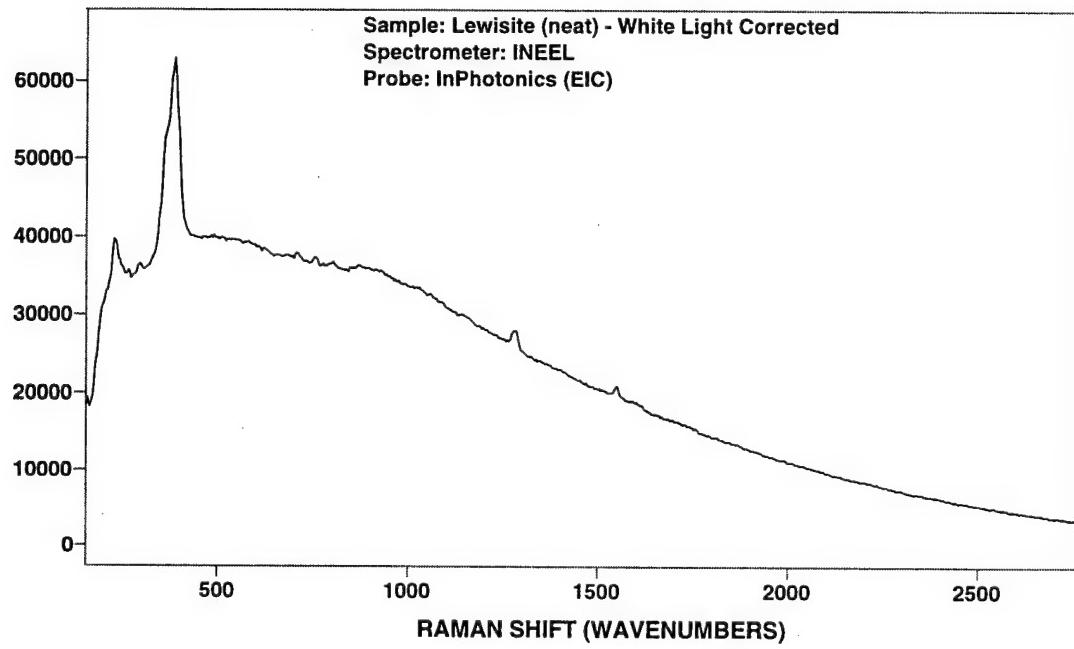


Figure A- 14: Lewisite (neat) - InPhotonics Probe

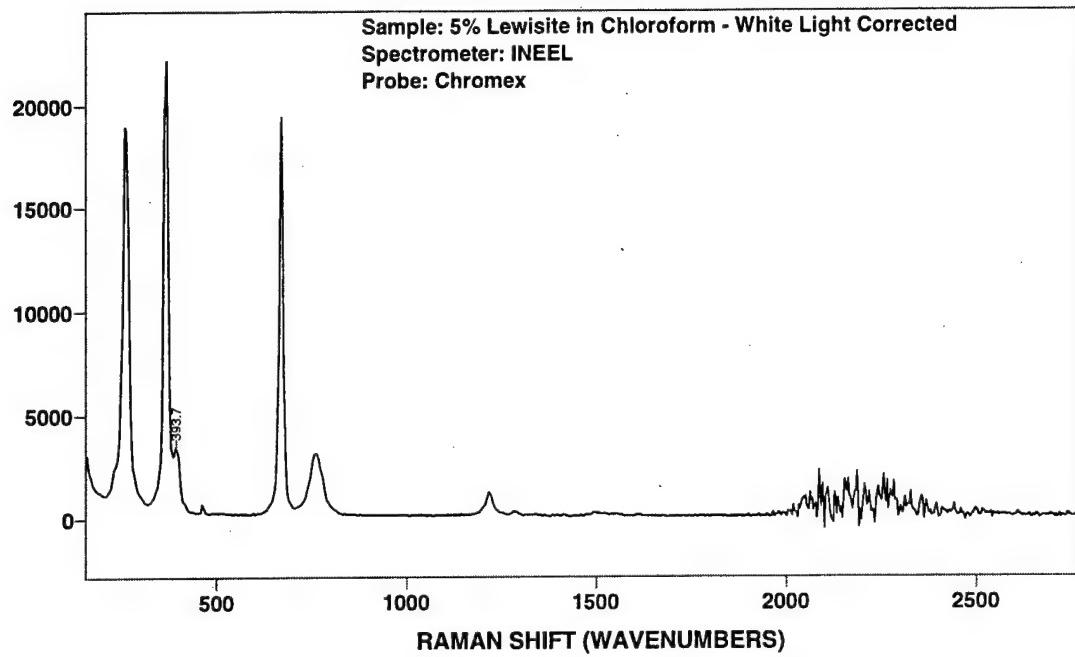


Figure A- 15: 5% Lewisite in Chloroform - Chromex Probe

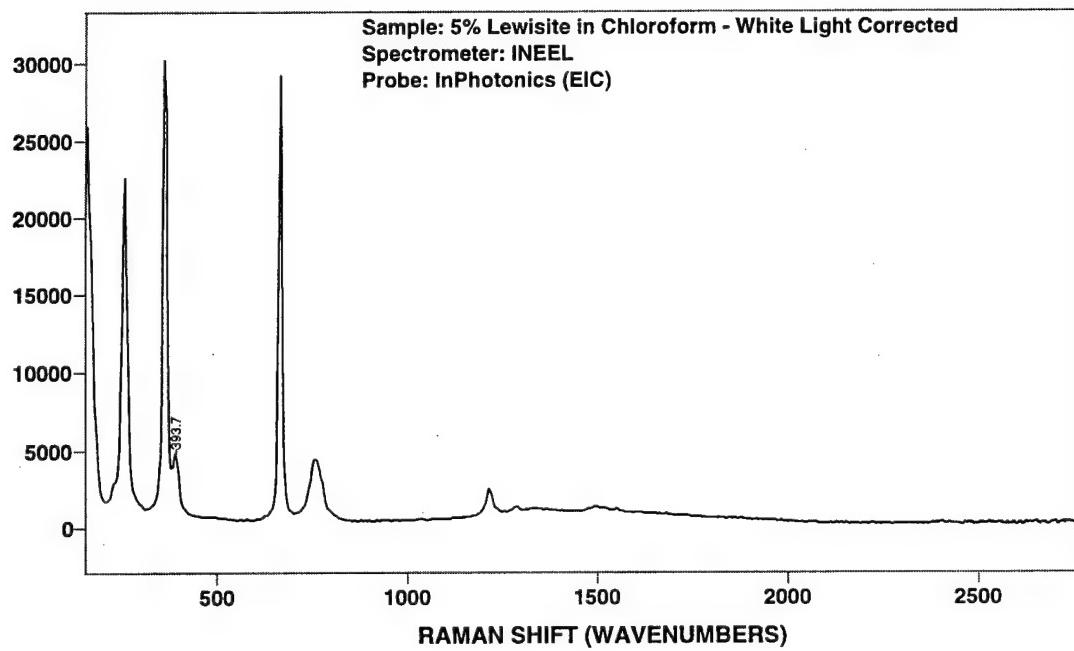


Figure A- 16: 5% Lewisite in Chloroform - InPhotonics Probe

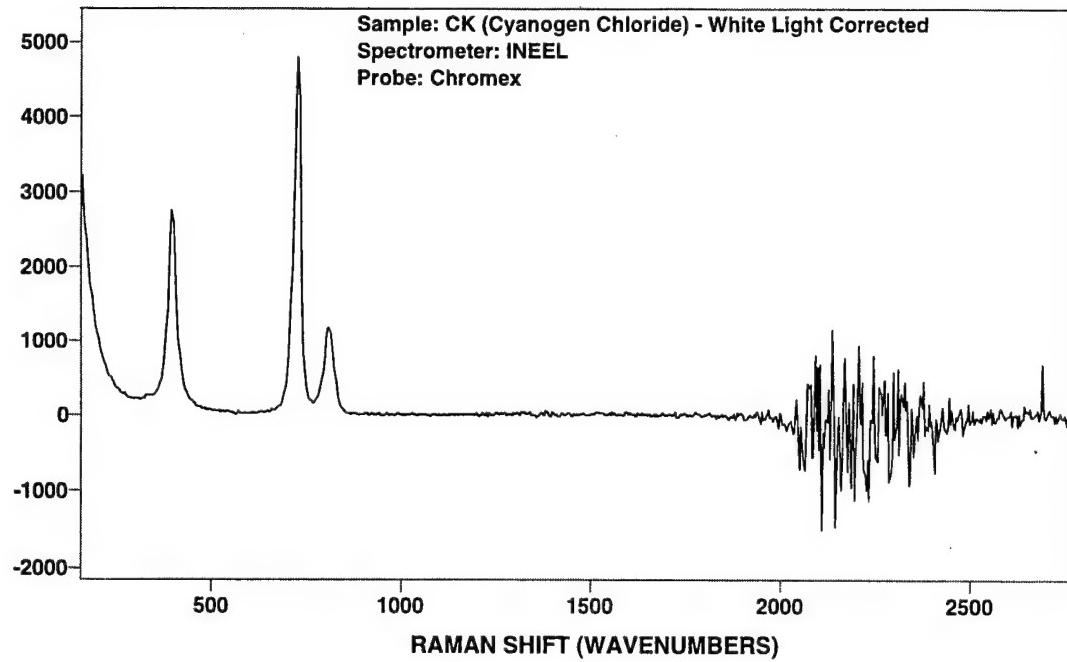


Figure A- 17: Cyanogen Chloride - Chromex Probe

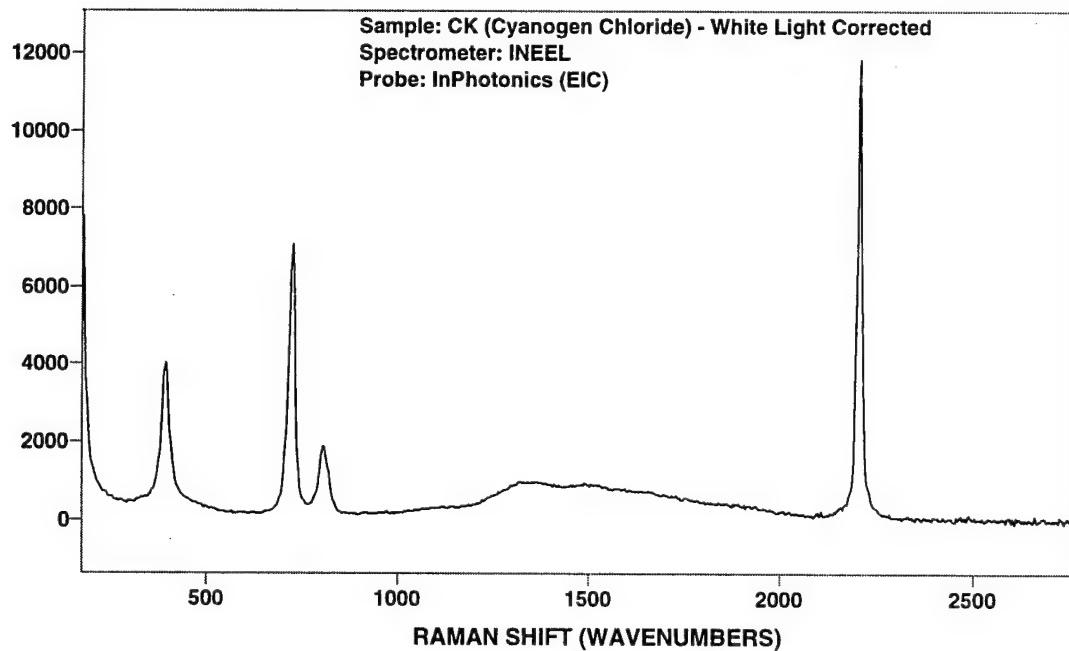


Figure A- 18: Cyanogen Chloride - InPhotonics Probe

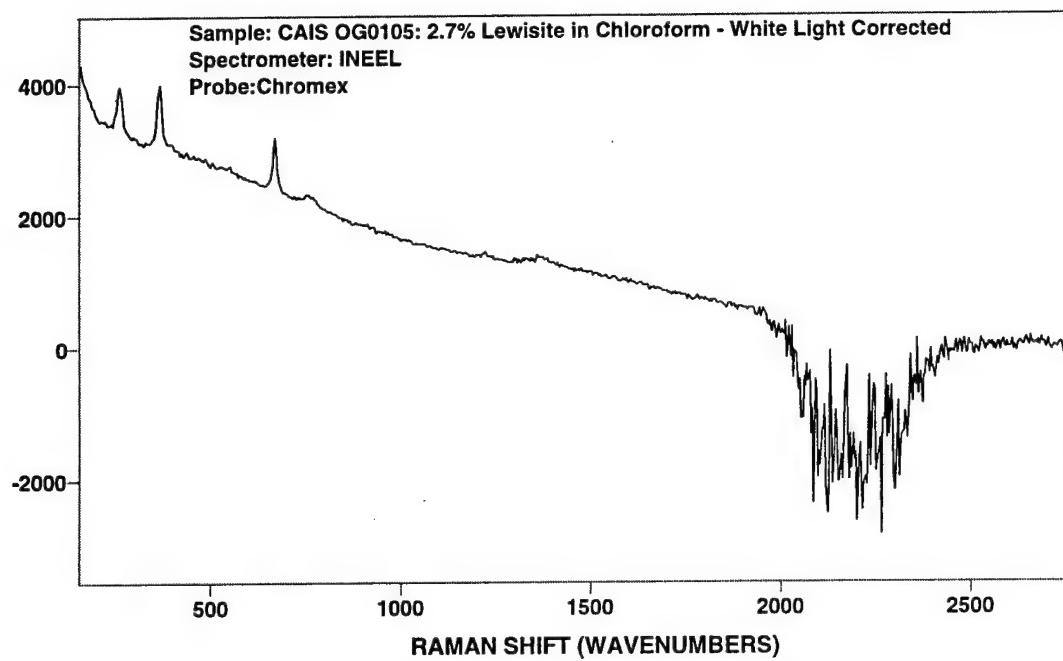


Figure A- 19: CAIS Item OG0105 - Chromex Probe

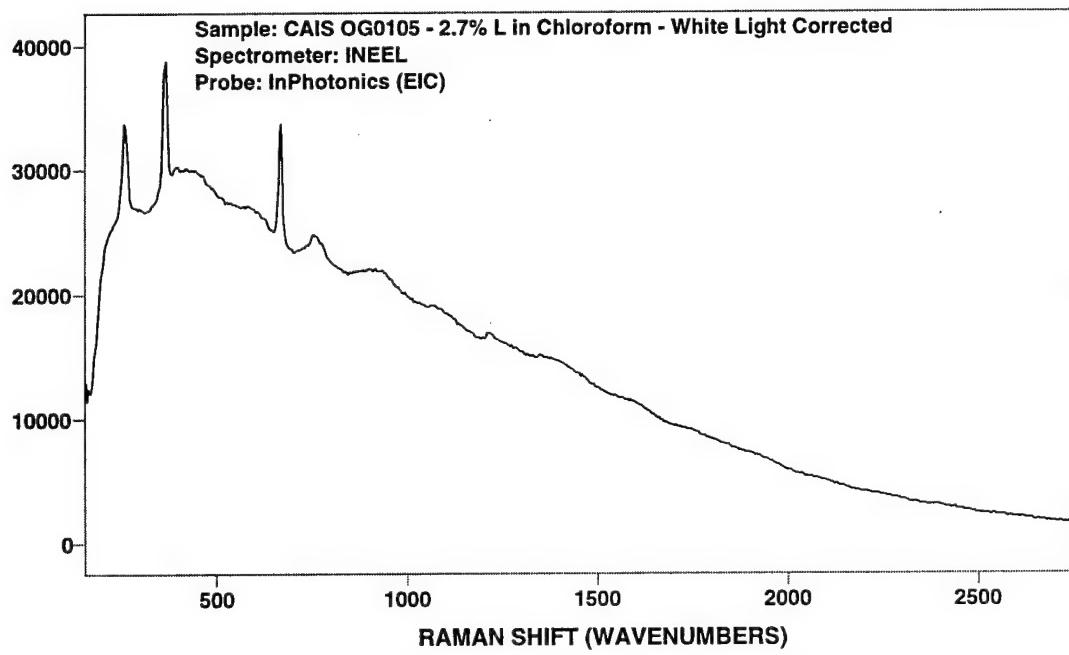


Figure A- 20: CAIS OG0105 - InPhotonics Probe

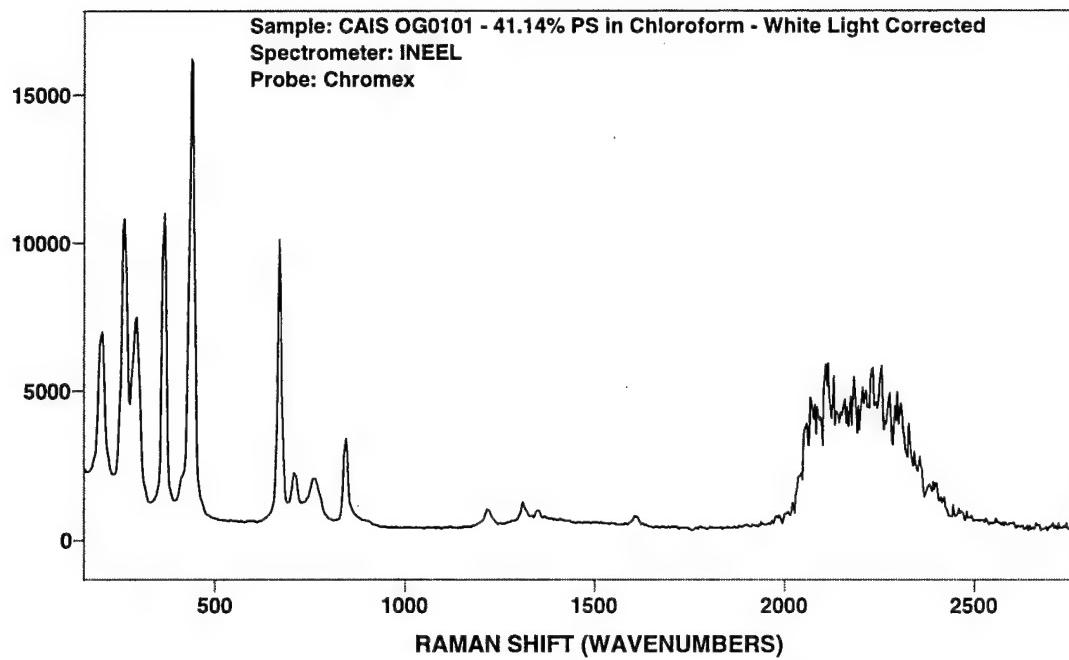


Figure A- 21: CAIS OG0101 - Chromex Probe

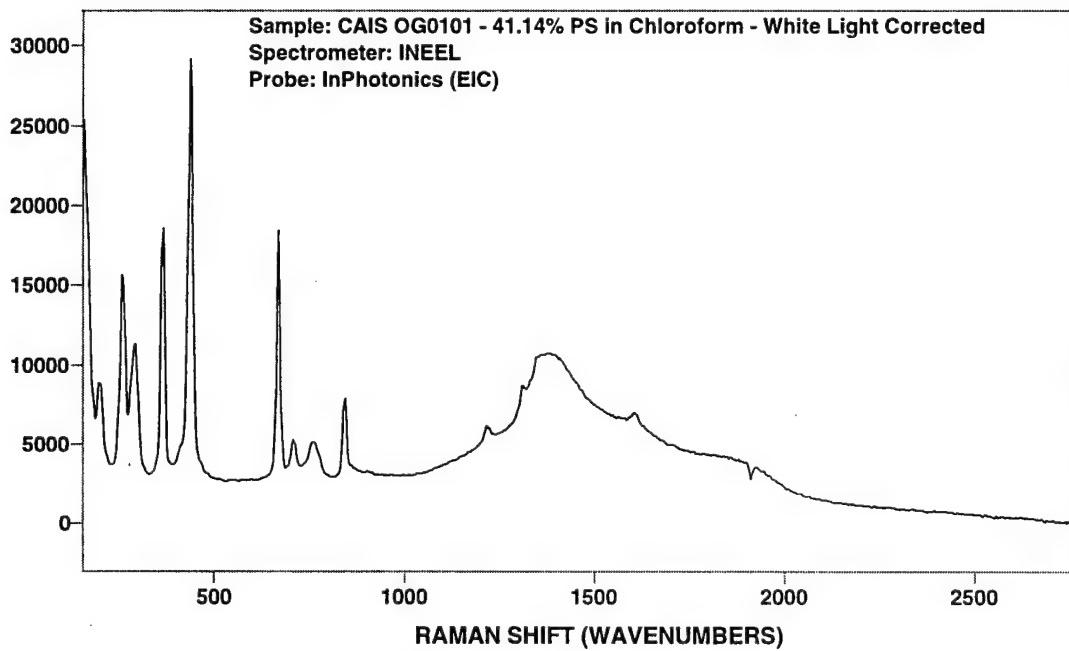


Figure A- 22: CAIS OG0101 - InPhotonics Probe

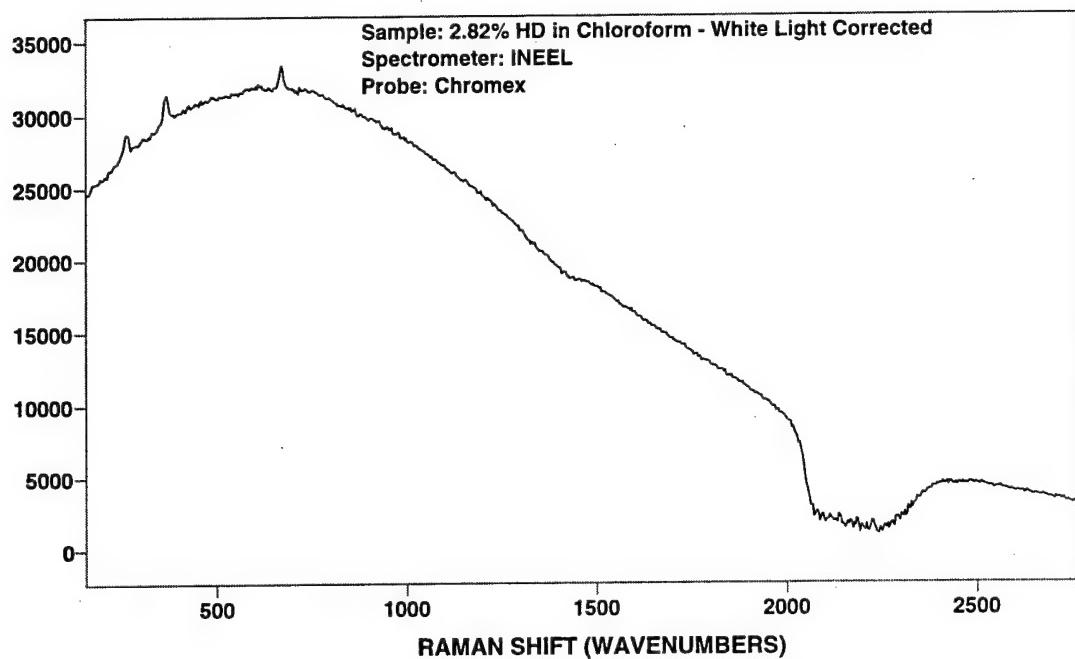


Figure A- 23: CAIS OG0207 - Chromex Probe

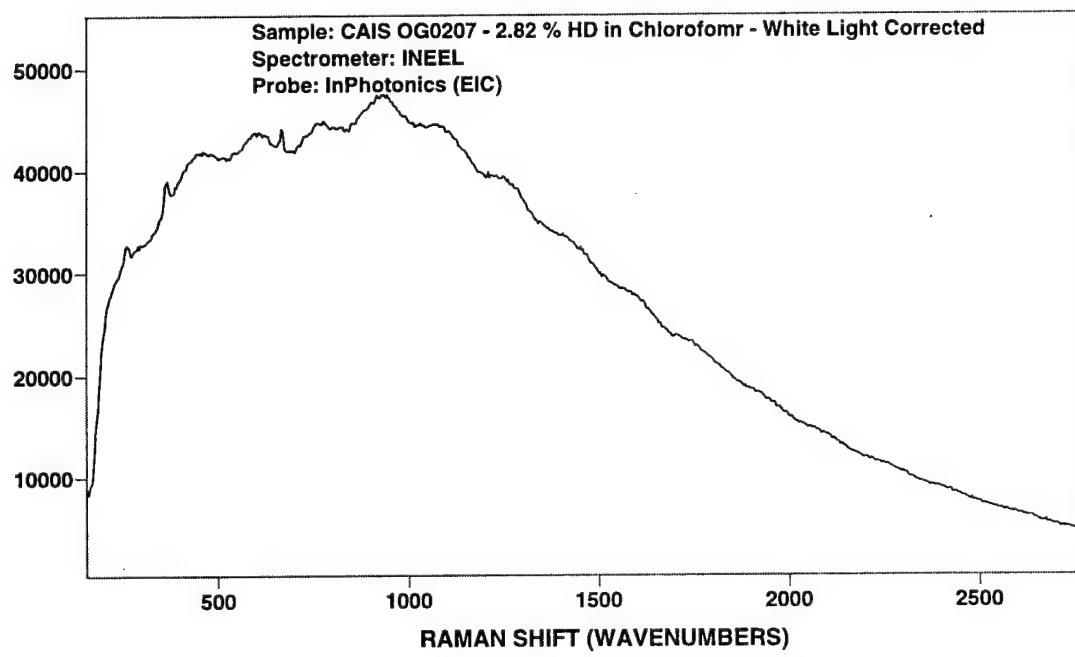


Figure A- 24: CAIS OG0207 - InPhotonics Probe

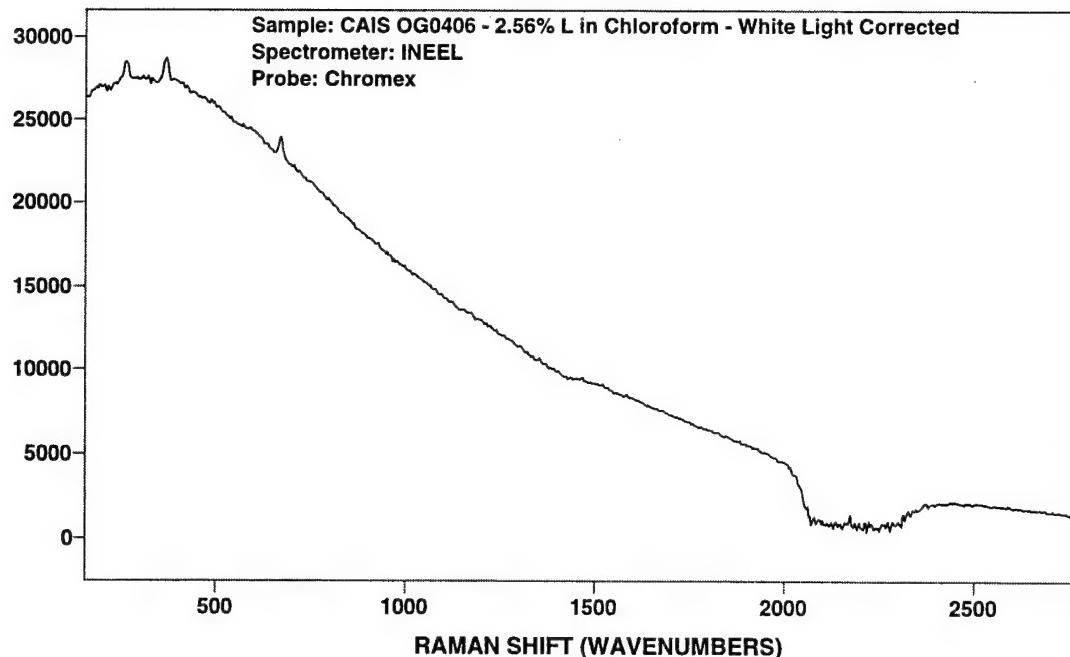


Figure A- 25: CAIS OG0406 - Chromex Probe

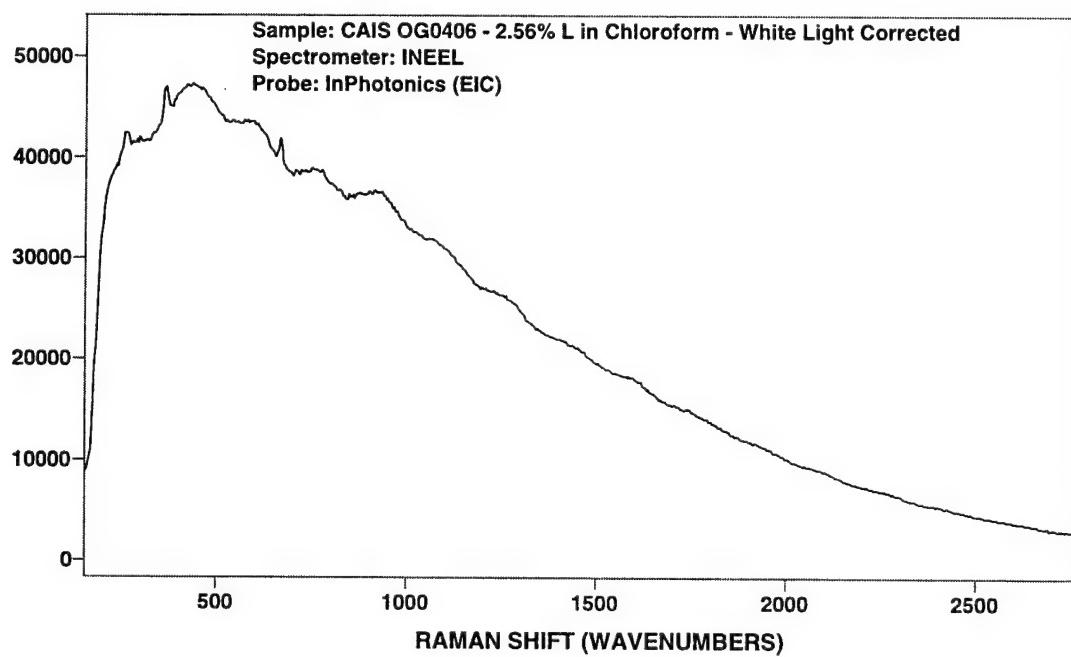


Figure A- 26: CAIS OG0406 - InPhotonics Probe

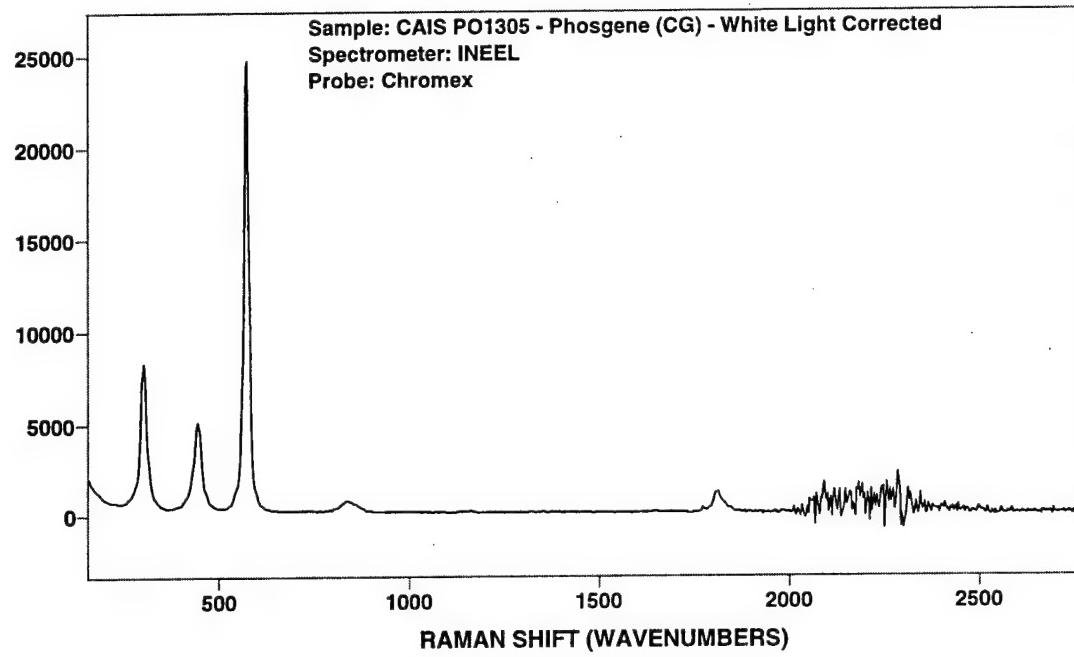


Figure A- 27: CAIS PO1305 - Chromex Probe

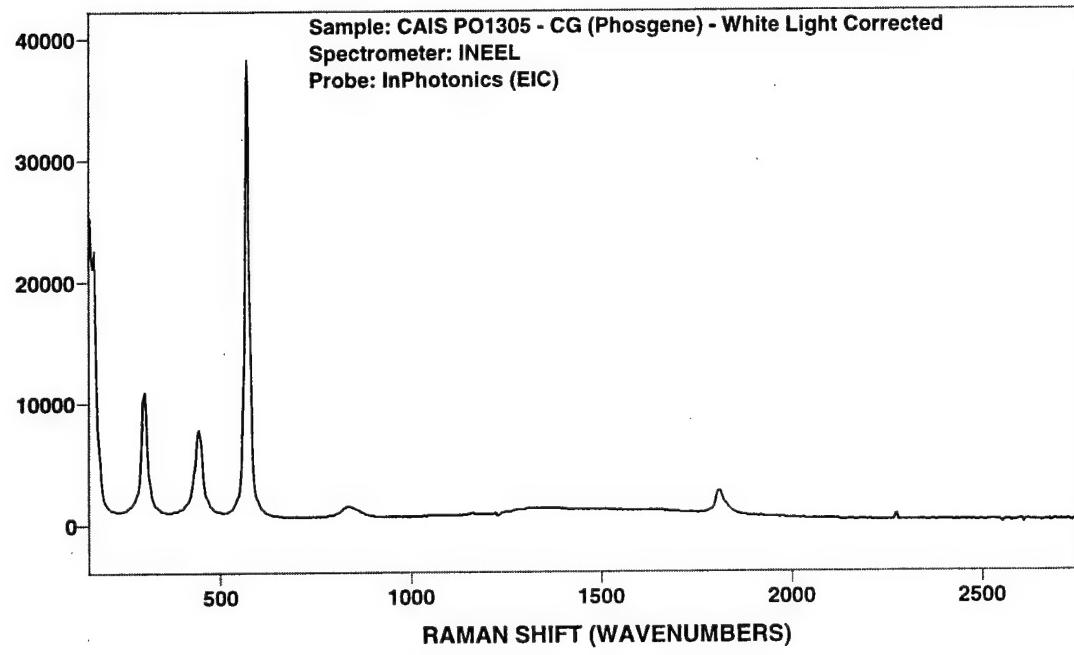


Figure A- 28: CAIS PO1305 - InPhotonics Probe

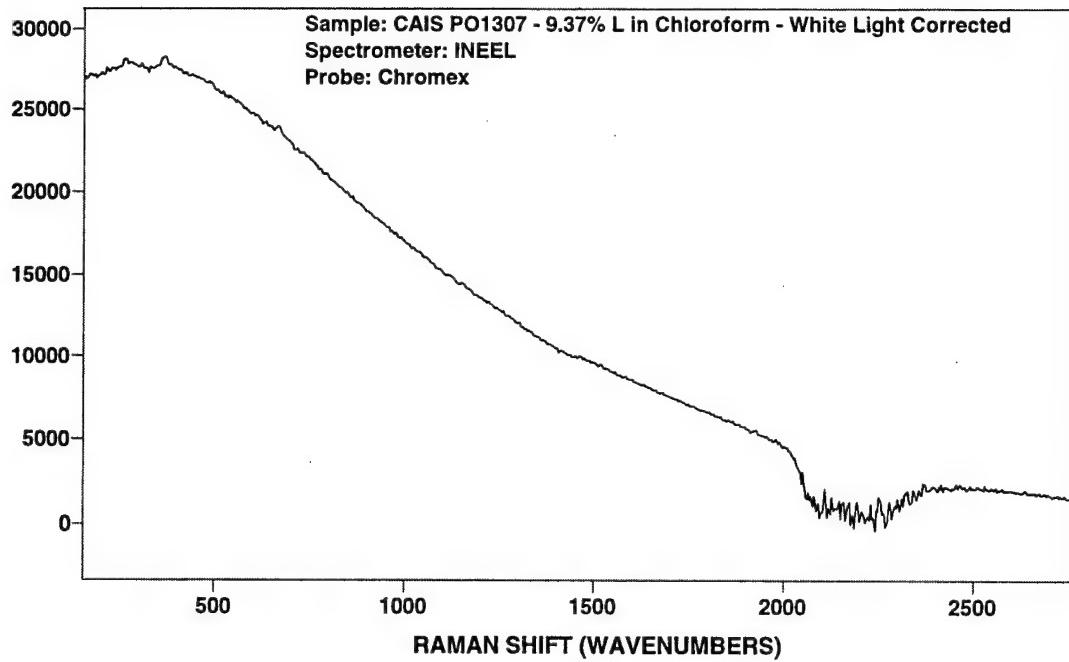


Figure A- 29: CAIS PO1307 - Chromex Probe

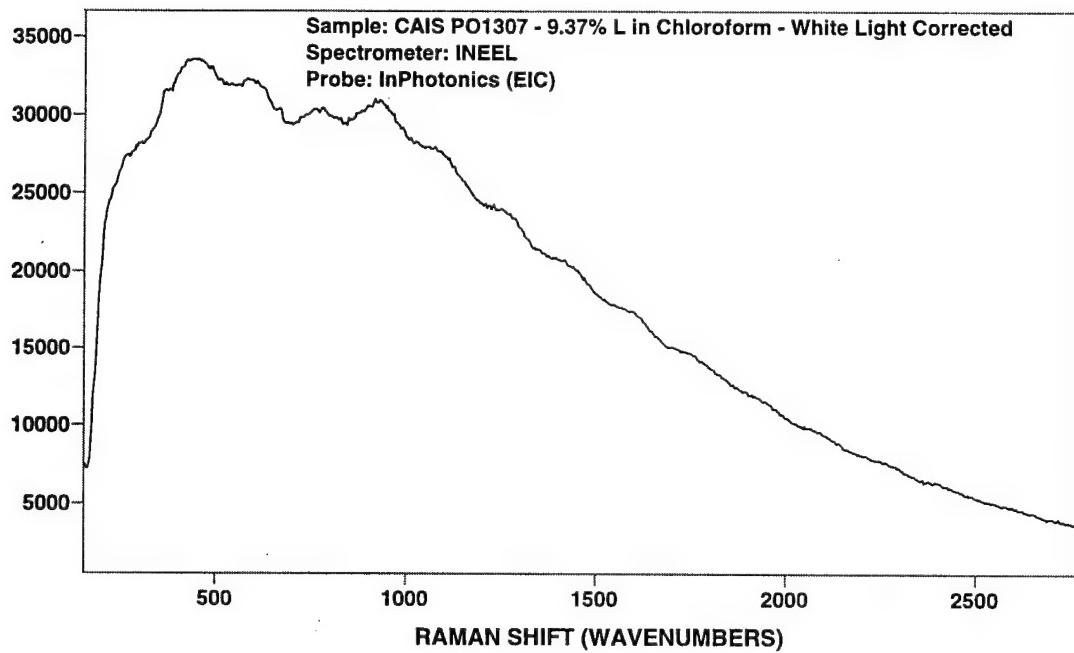


Figure A- 30: CAIS PO1307 - InPhotonics Probe

APPENDIX B: Spectra Obtained with the InPhotote Raman System.

FIGURES

B- 1: Adamsite (DM)	36
B- 2: Chloroacetophenone (CN). Inset spectrum has been baseline corrected.....	36
B- 3: 50% Chloropicrin in Chloroform.....	37
B- 4: Mustard (HD).....	37
B- 5: 5% HD in Chloroform.....	38
B- 6: Nitrogen Mustard (HN-1)	38
B- 7: Lewisite (L).....	39
B- 8: Lewisite (5%) in chloroform.....	39
B- 9: CAIS item OG0101 (chloropicrin in chloroform)	40
B- 10: CAIS item OG0105 (lewisite in chloroform).....	40
B- 11: CAIS item OG0207 (mustard in chloroform)	41
B- 12: CAIS item OG0406 (lewisite in chloroform).....	41
B- 13: CAIS item PO1305 (phosgene).....	42
B- 14: CAIS item PO1307 (lewisite in chloroform)	42

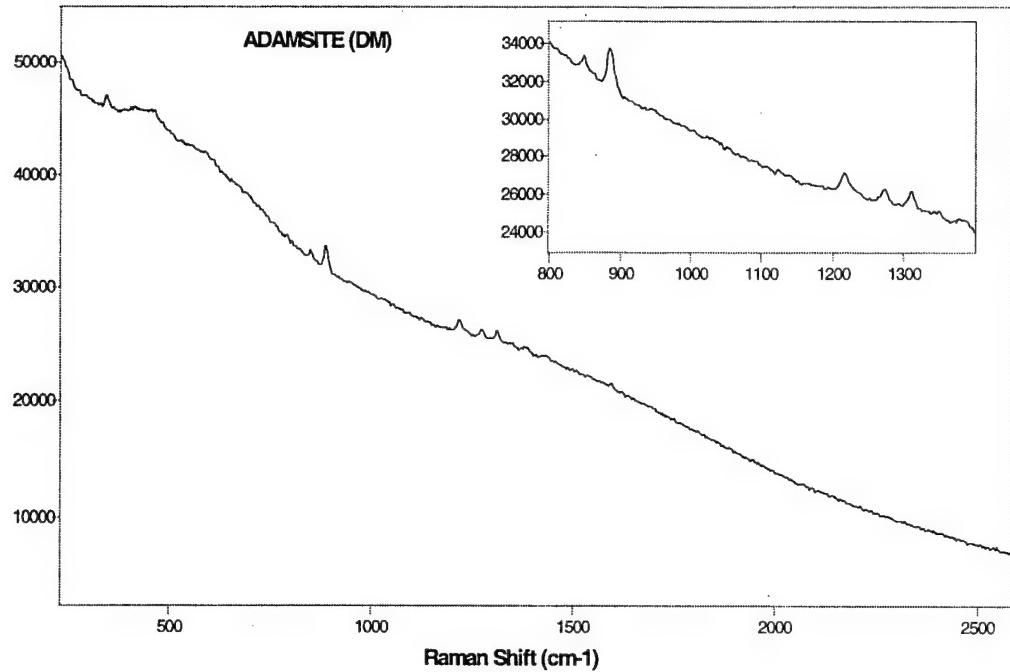


Figure B- 1: Adamsite (DM)

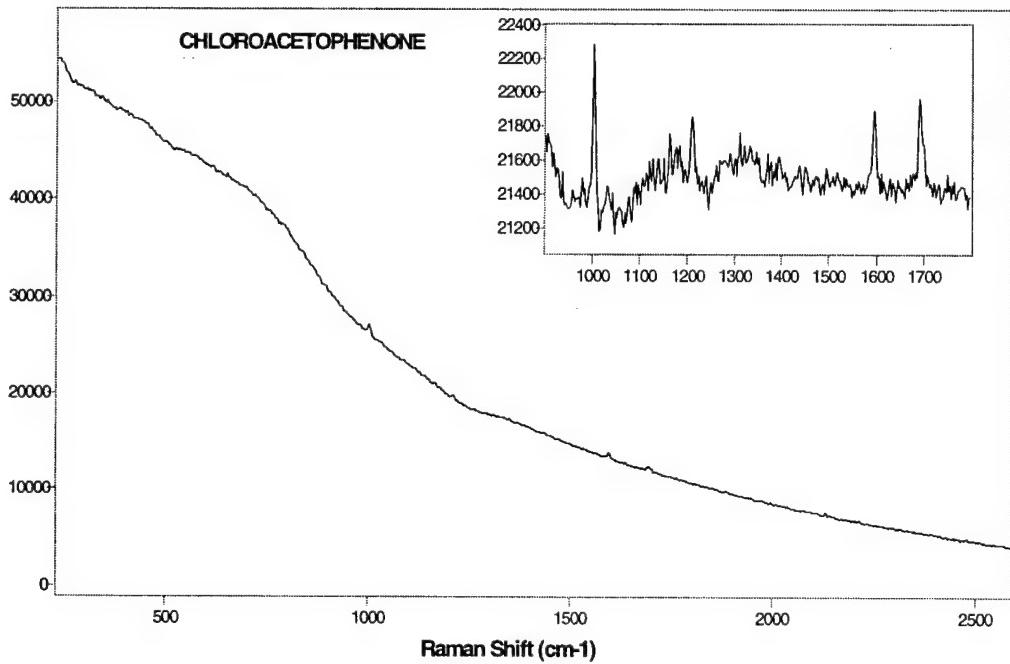


Figure B- 2: Chloroacetophenone (CN). Inset spectrum has been baseline corrected.

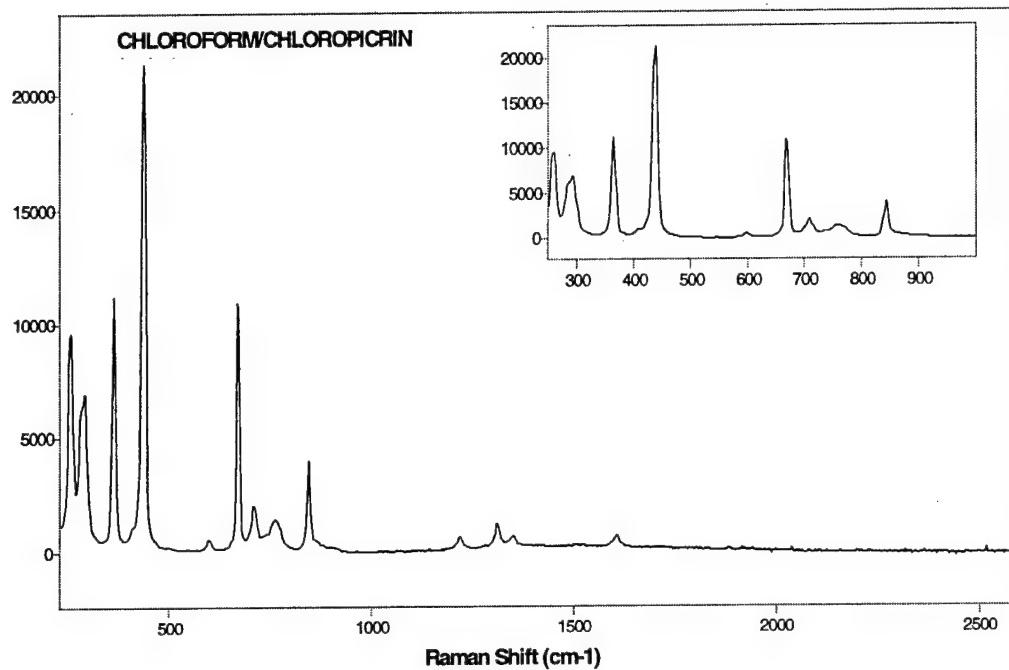


Figure B- 3: 50% Chloropicrin in Chloroform

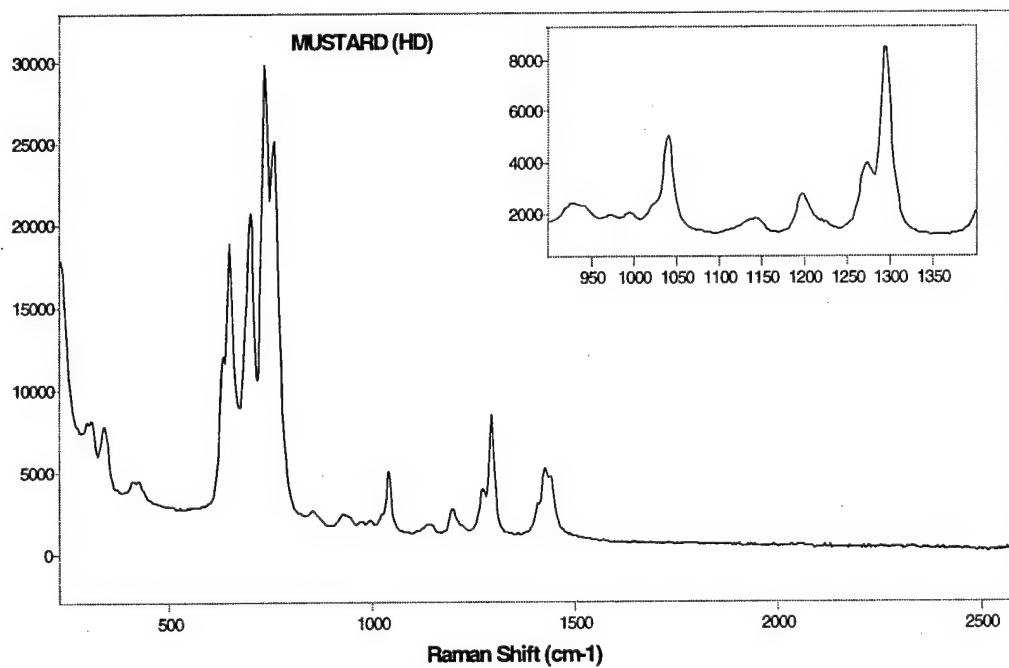


Figure B- 4: Mustard (HD)

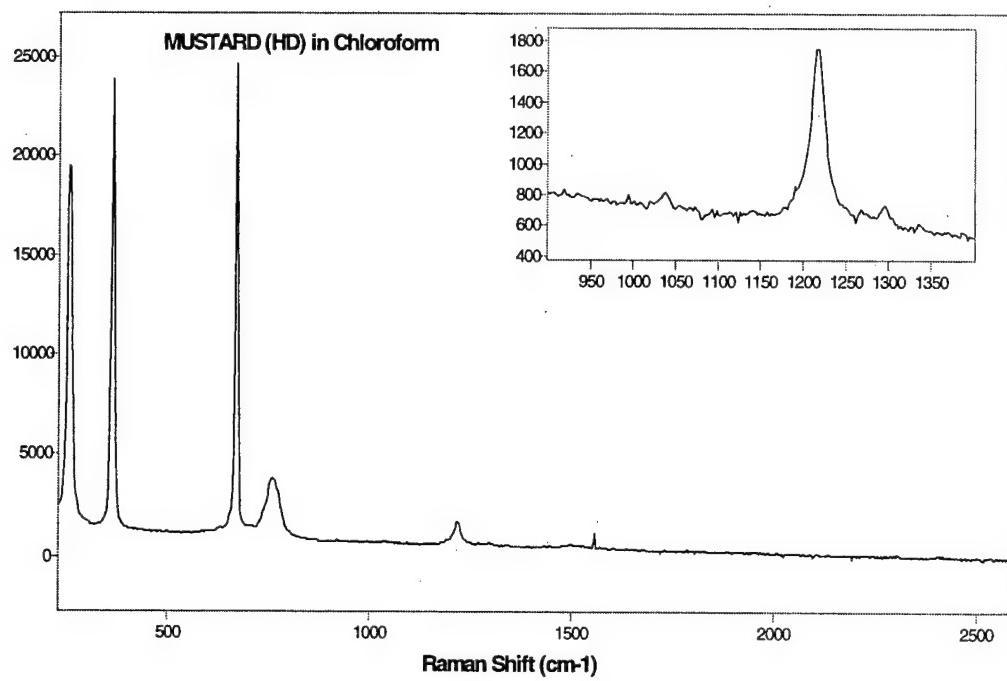


Figure B- 5: 5% HD in Chloroform

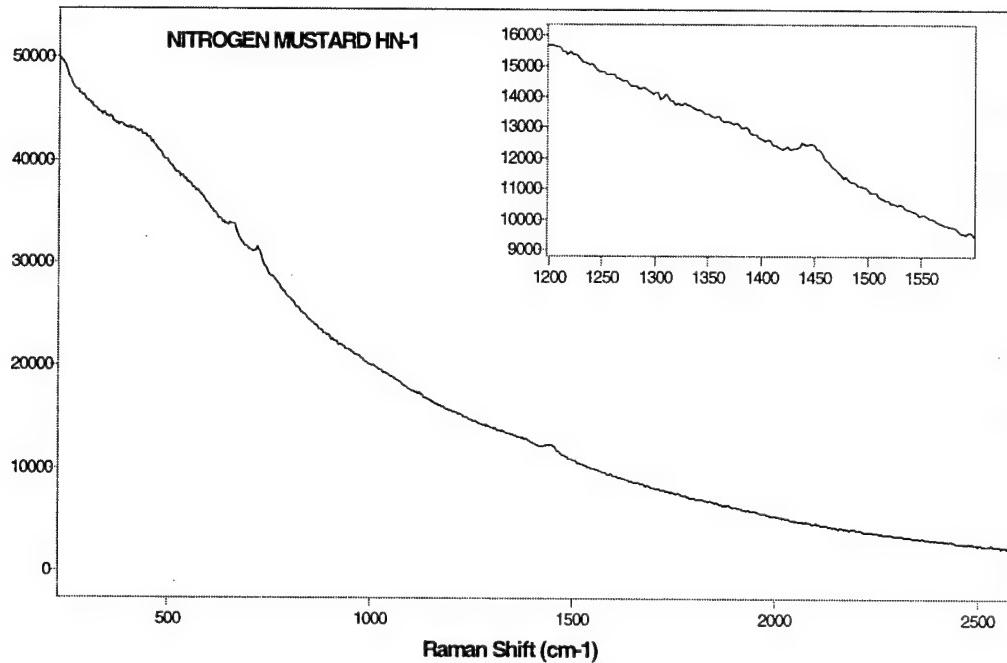


Figure B- 6: Nitrogen Mustard (HN-1)

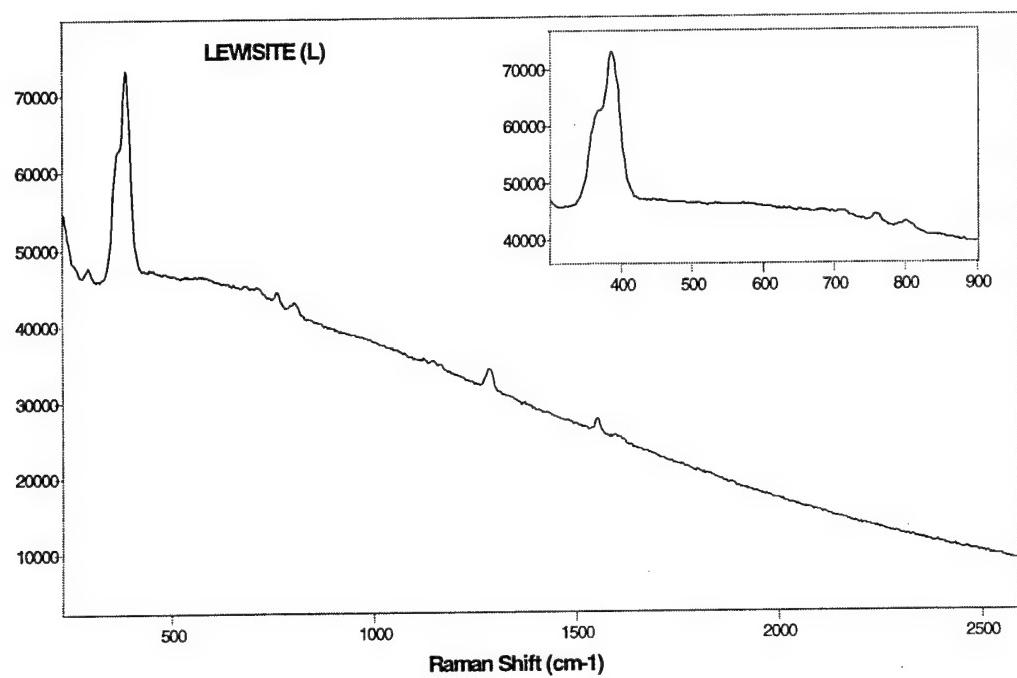


Figure B- 7: Lewisite (L)

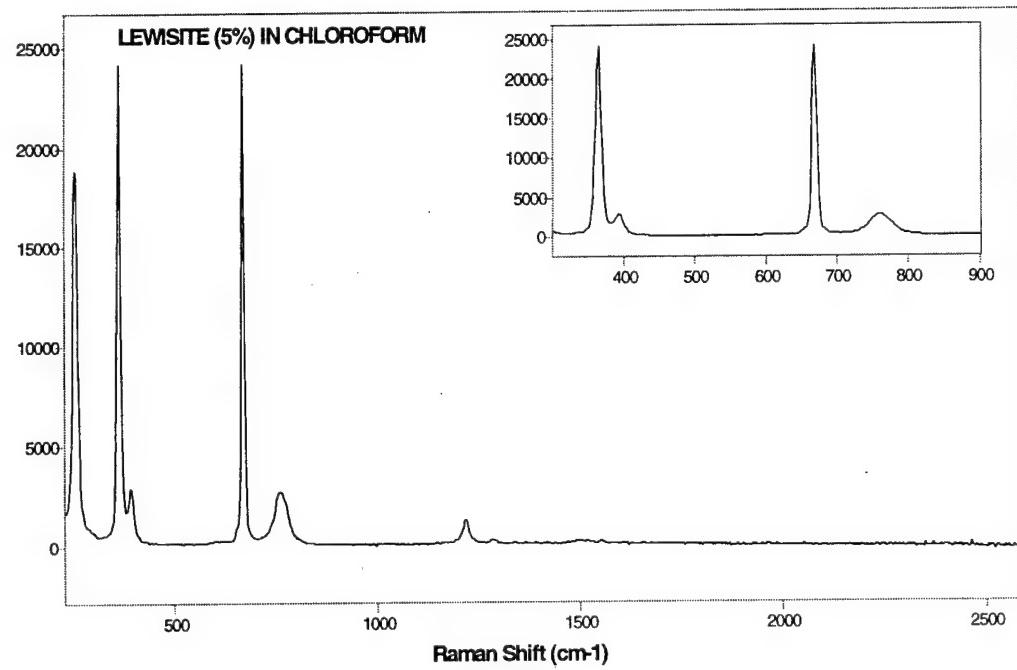


Figure B- 8: Lewisite (5 %) in chloroform

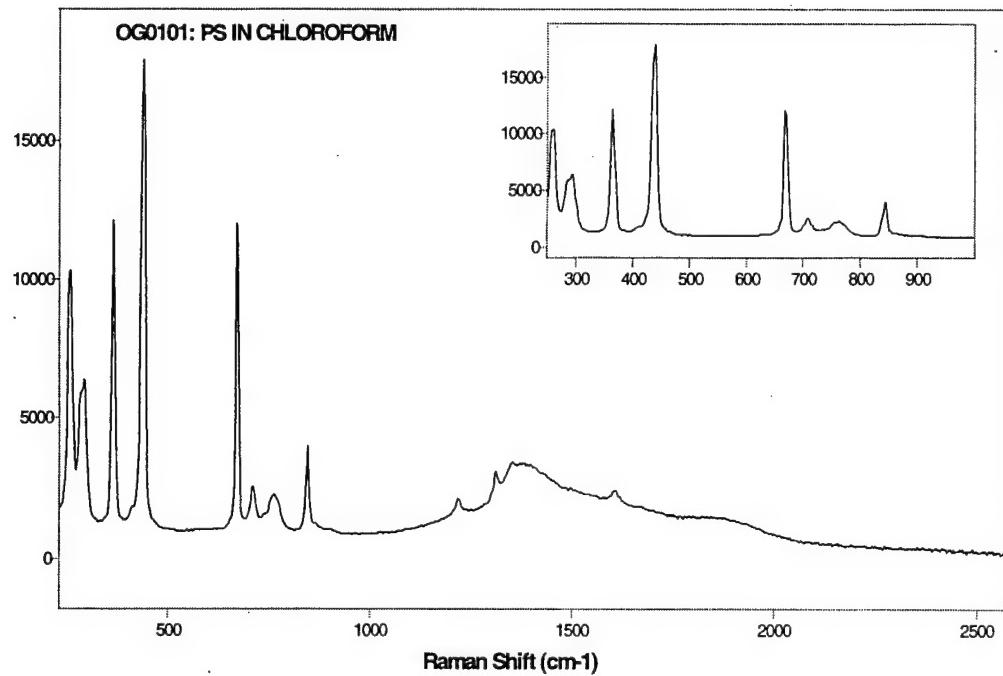


Figure B- 9: CAIS item OG0101 (chloropicrin in chloroform)

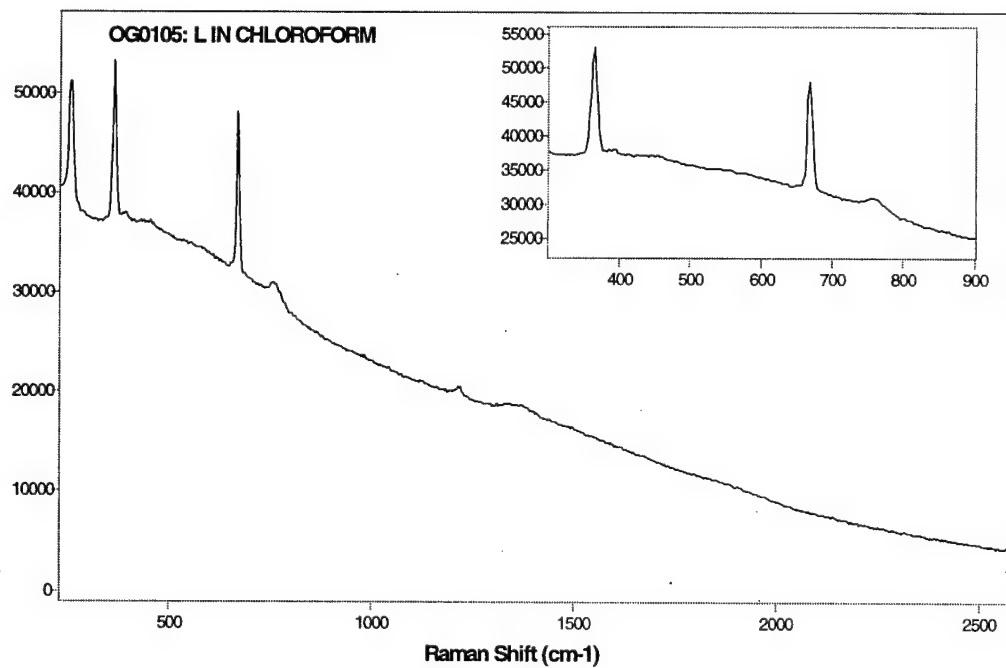


Figure B- 10: CAIS item OG0105 (lewisite in chloroform)

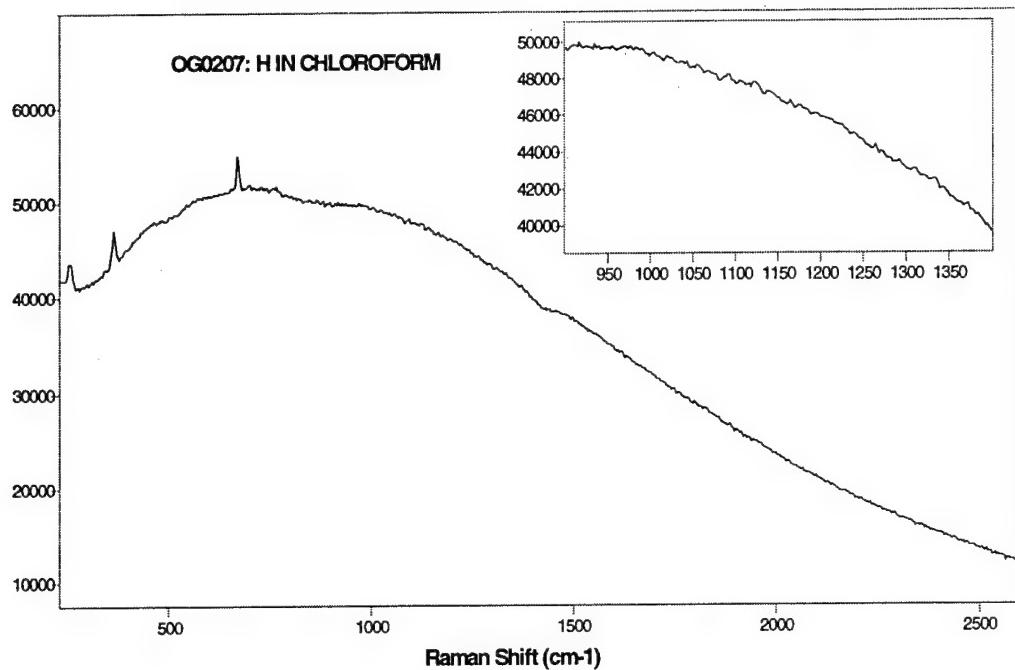


Figure B- 11: CAIS item OG0207 (mustard in chloroform)

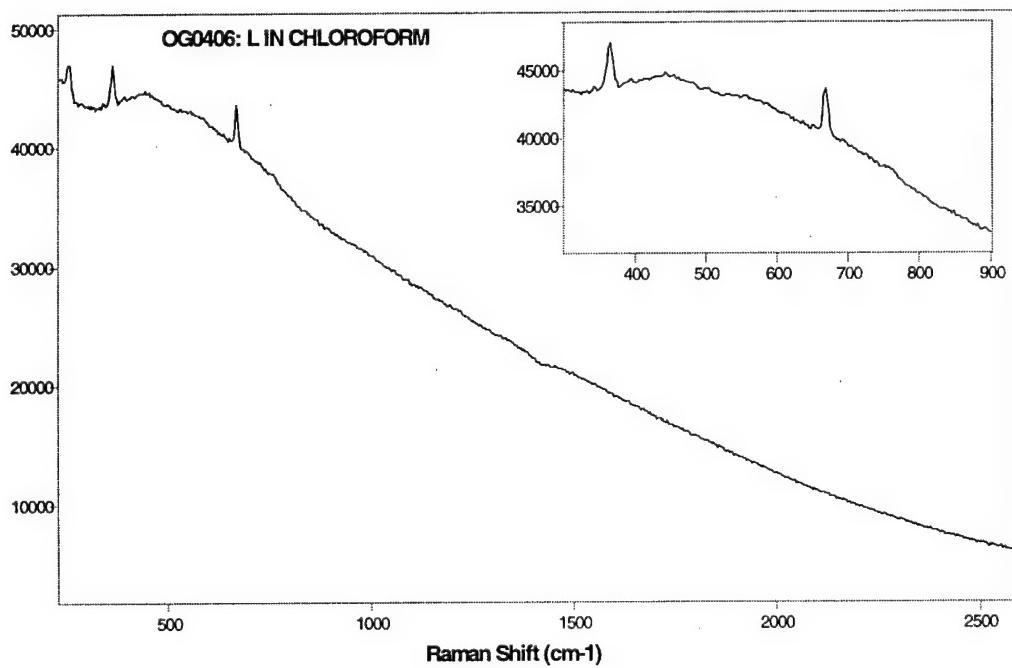


Figure B- 12: CAIS item OG0406 (lewisite in chloroform)

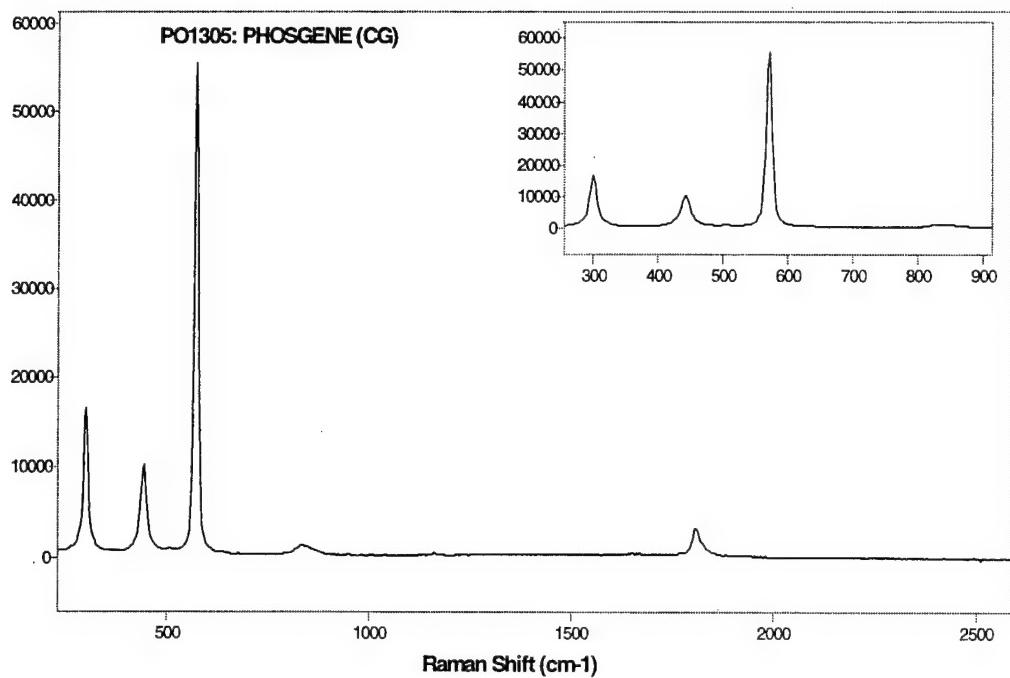


Figure B- 13: CAIS item PO1305 (phosgene)

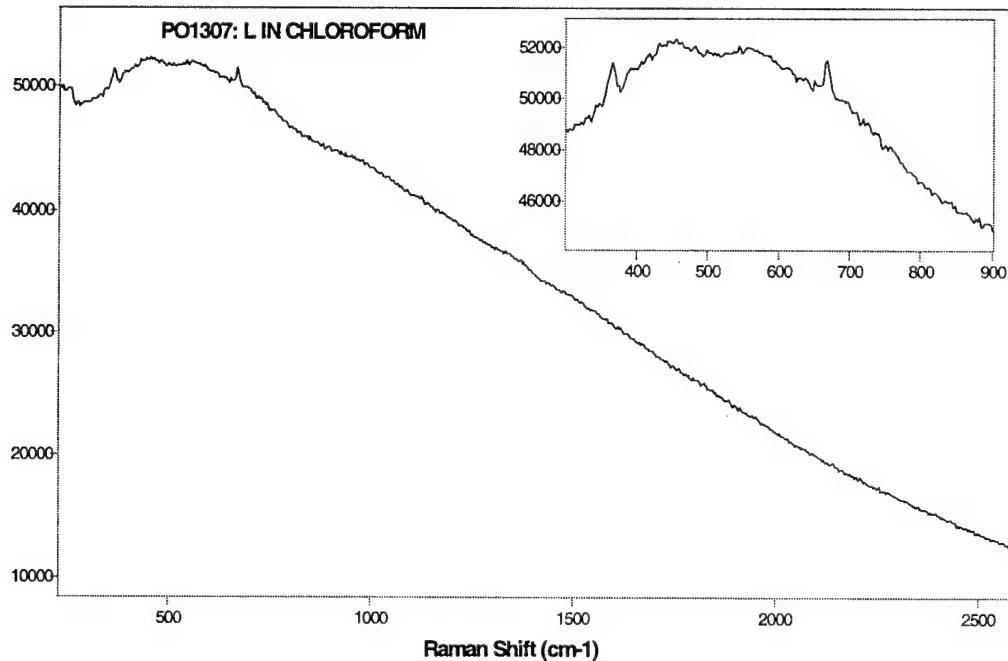


Figure B- 14: CAIS item PO1307 (lewisite in chloroform)

APPENDIX C: Spectra Obtained with the Sentinel Raman System.

FIGURES

C- 1: Adamsite (DM)	44
C- 2: Chloroacetophenone (CN)	44
C- 3: 50% Chloropicrin in Chloroform	45
C- 4: Mustard (HD)	45
C- 5: 5% HD in Chloroform.....	46
C- 6: Nitrogen Mustard HN-1	46
C- 7: Lewisite (L).....	47
C- 8: Lewisite (5%) in chloroform.....	47
C- 9: CAIS item OG0101 (chloropicrin in chloroform)	48
C- 10: CAIS item OG0105 (lewisite in chloroform).....	48
C- 11: CAIS item OG0207 (mustard in chloroform)	49
C- 12: CAIS item OG0406 (lewisite in chloroform).....	49
C- 13: CAIS item PO1305 (phosgene).....	50
C- 14: CAIS item PO1307 (lewisite in chloroform)	50

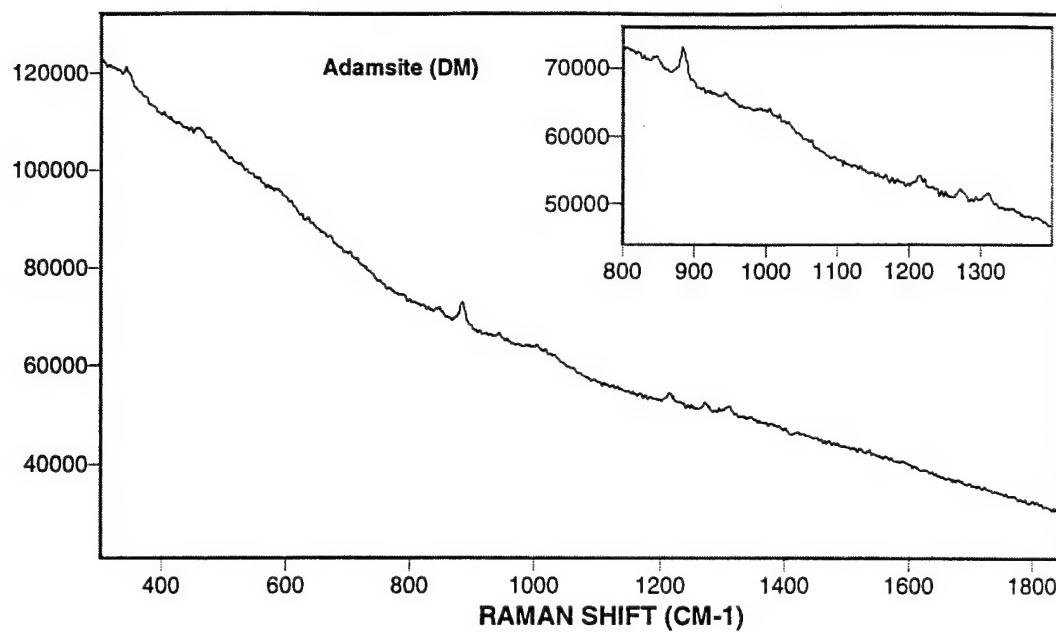


Figure C- 1: Adamsite (DM)

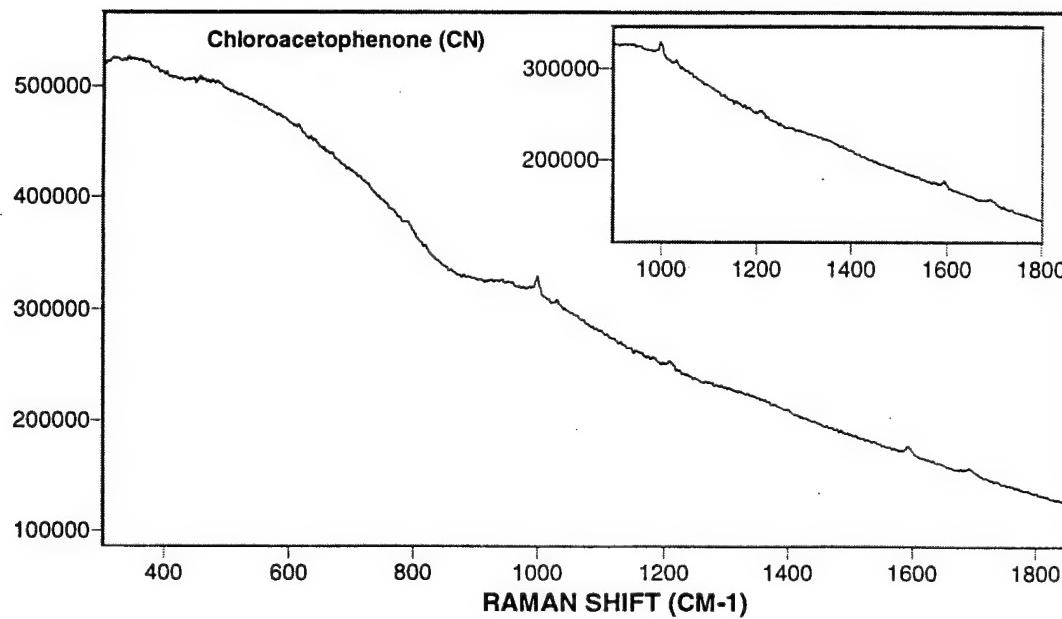


Figure C- 2: Chloroacetophenone (CN)

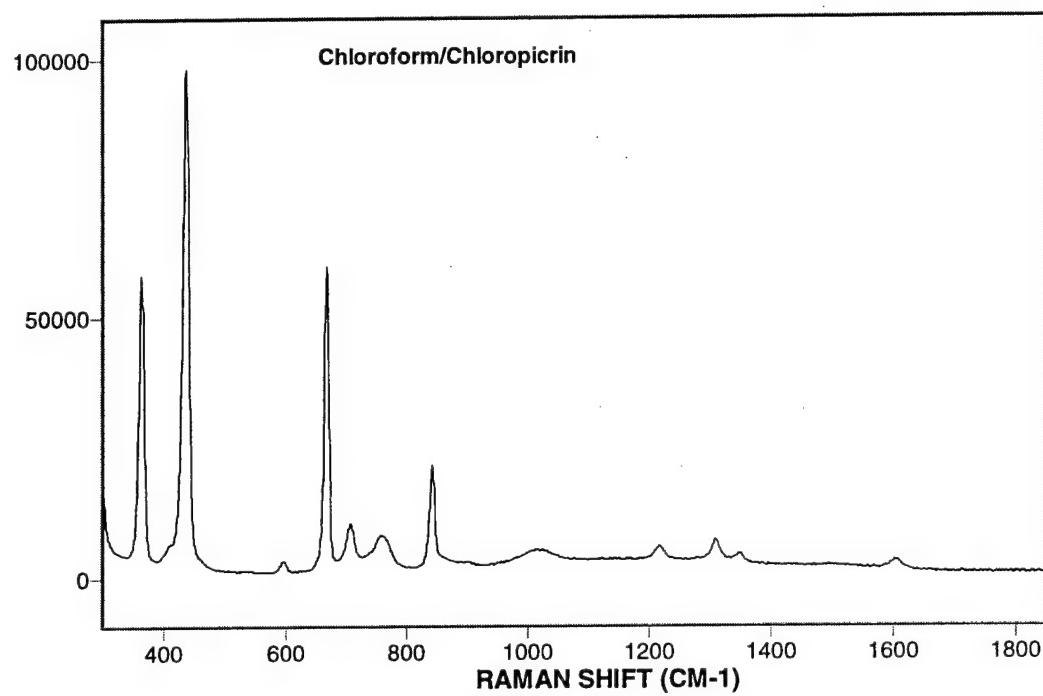


Figure C- 3: 50% Chloropicrin in Chloroform

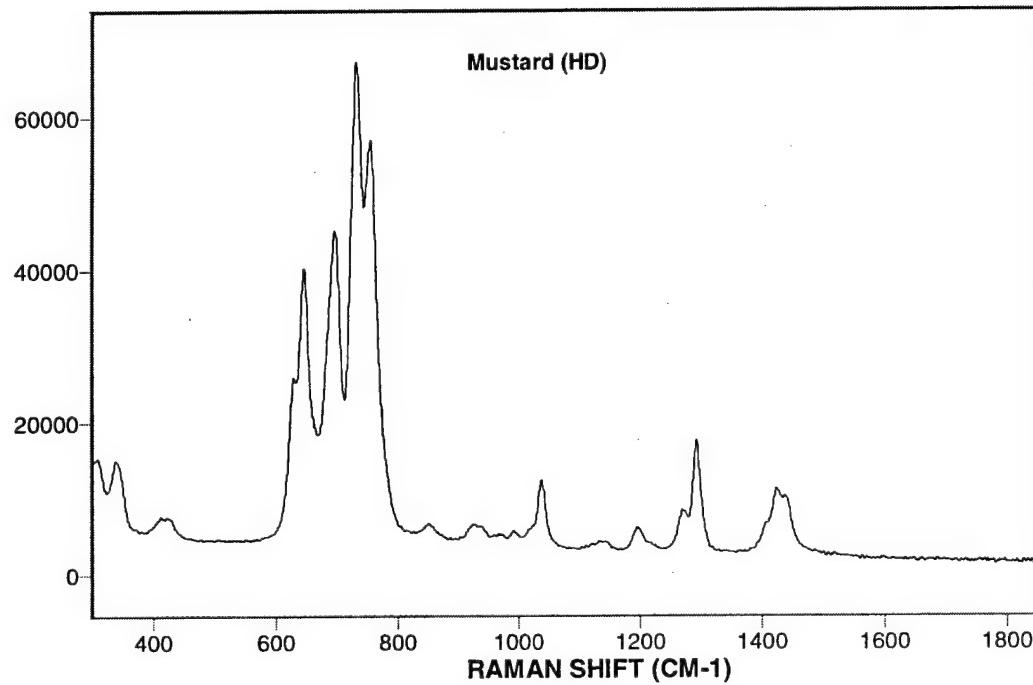


Figure C- 4: Mustard (HD)

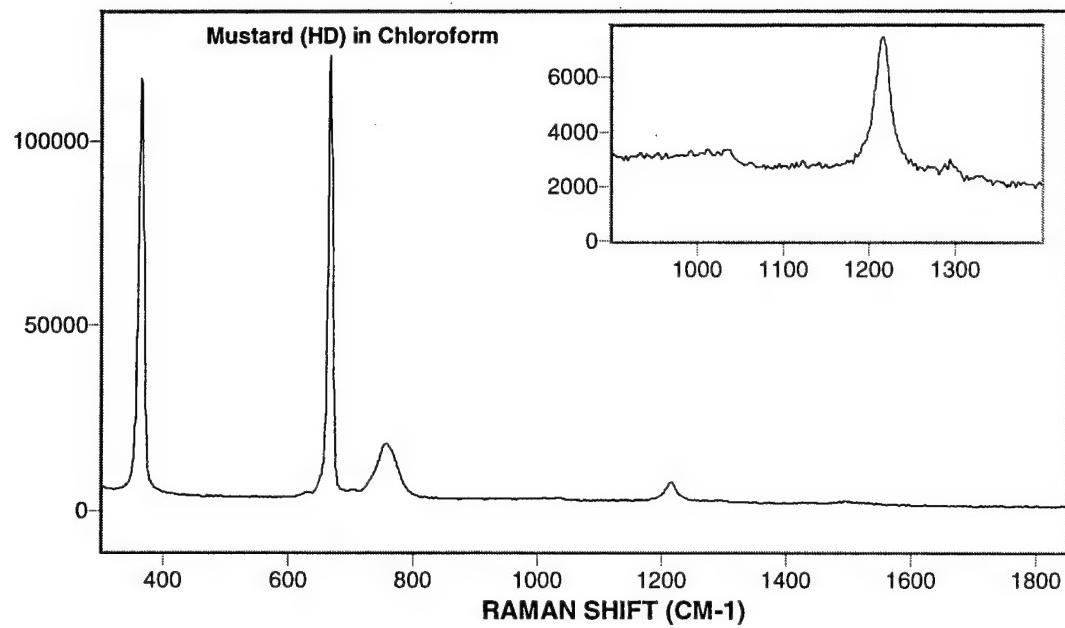


Figure C- 5: 5% HD in Chloroform

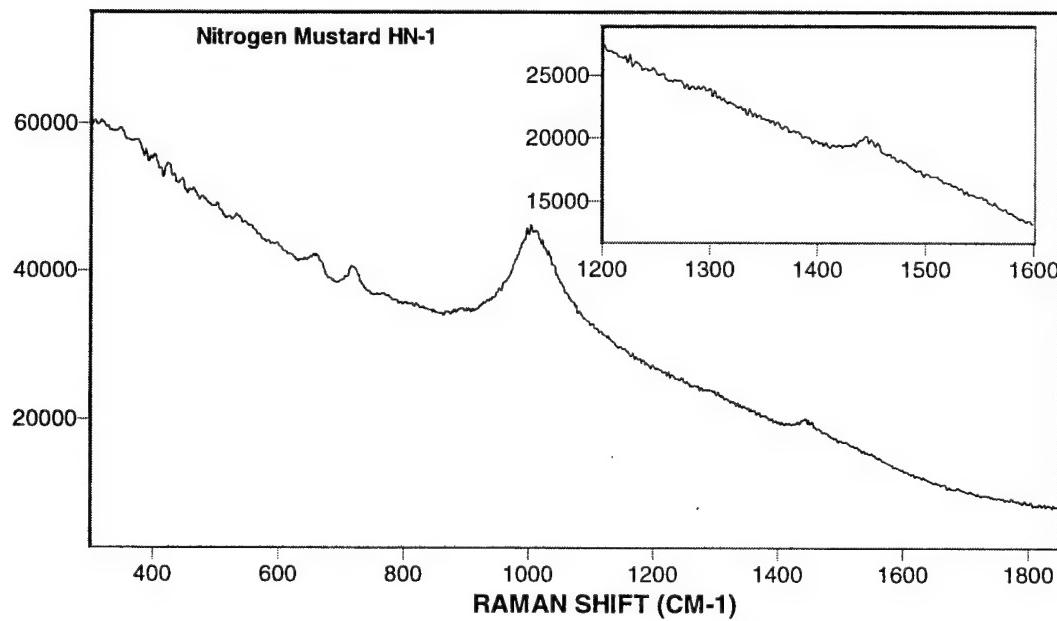


Figure C- 6: Nitrogen Mustard HN-1

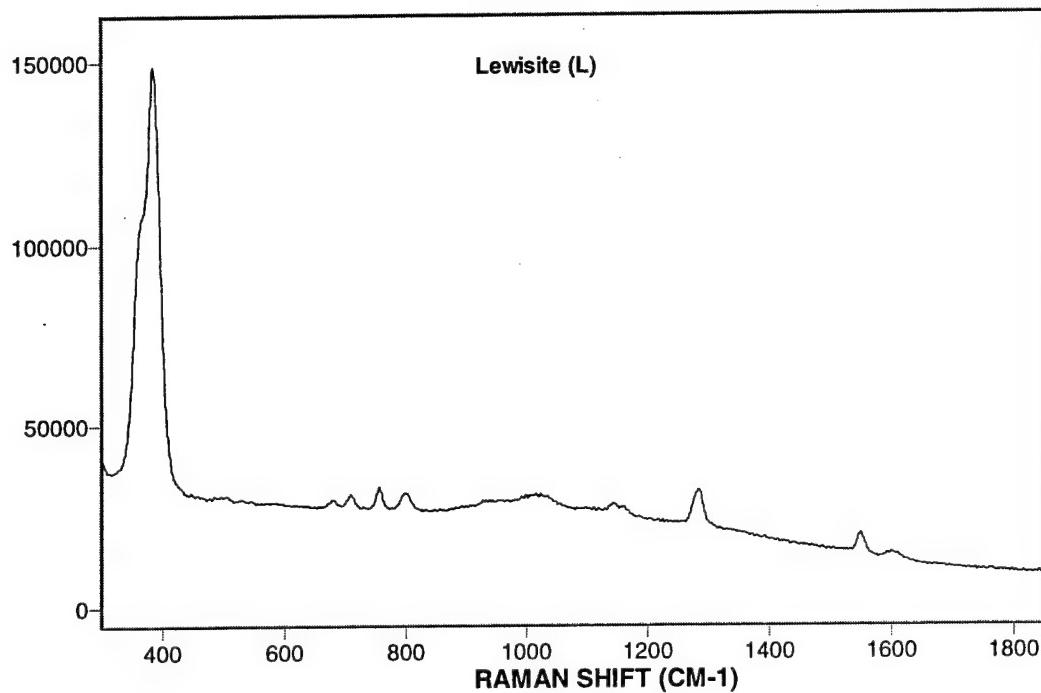


Figure C- 7: Lewisite (L)

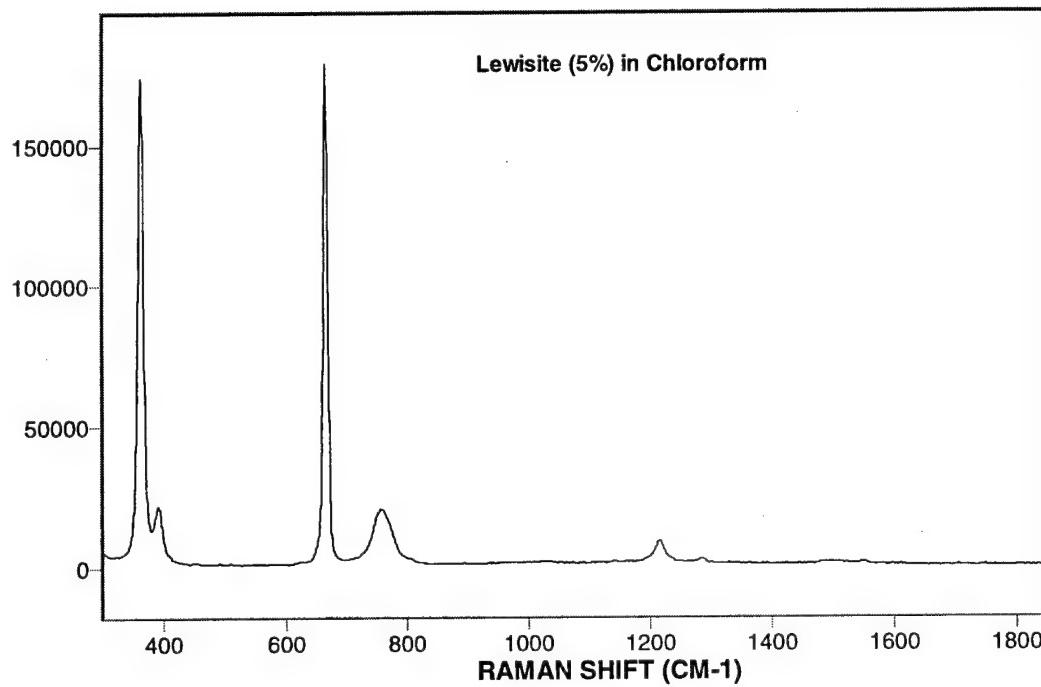


Figure C- 8: Lewisite (5%) in chloroform

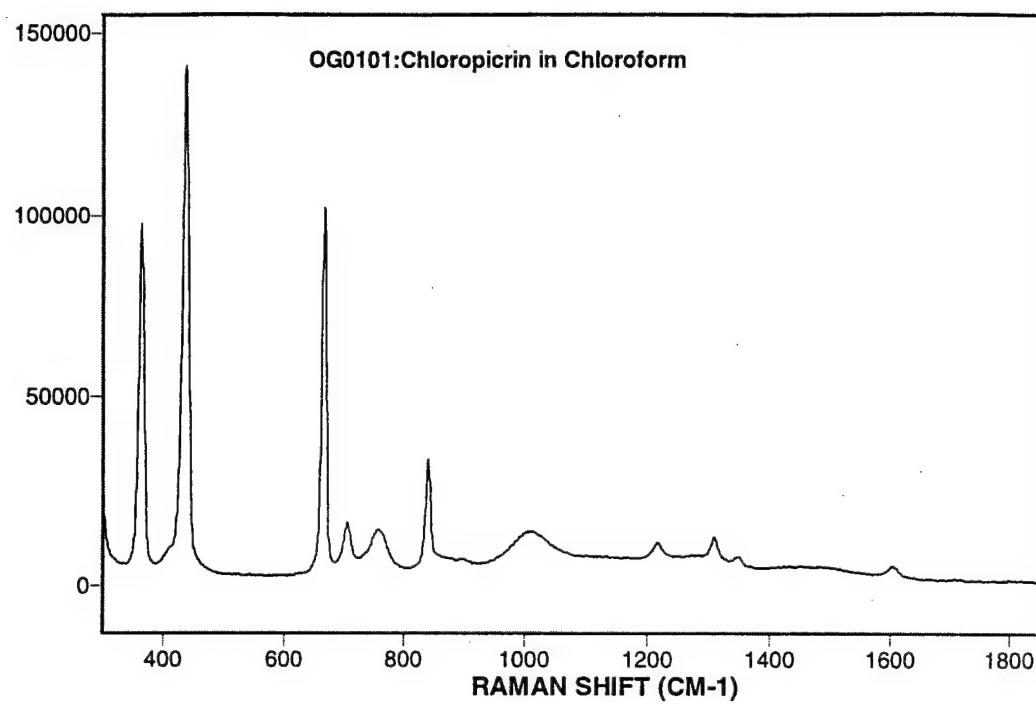


Figure C- 9: CAIS item OG0101 (chloropicrin in chloroform)

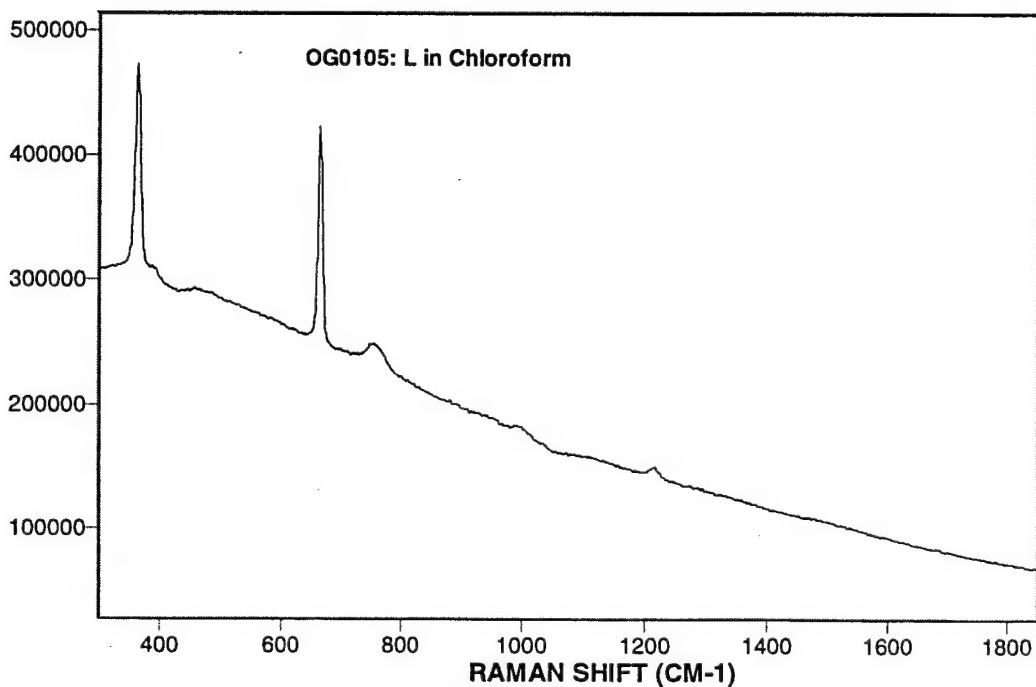


Figure C- 10: CAIS item OG0105 (lewisite in chloroform)

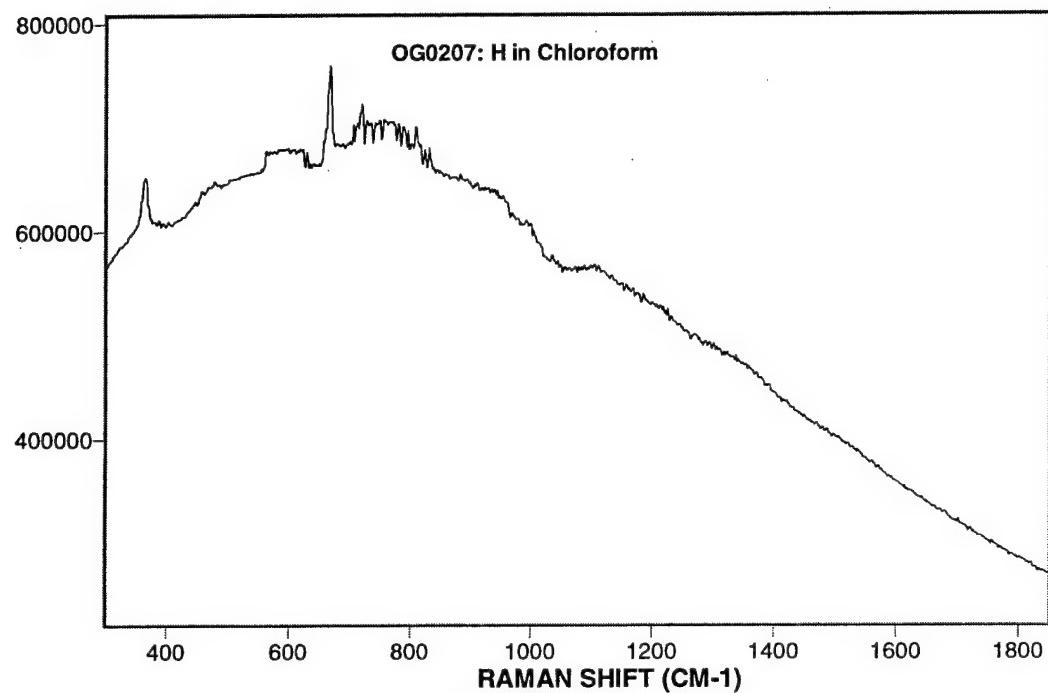


Figure C- 11: CAIS item OG0207 (mustard in chloroform)

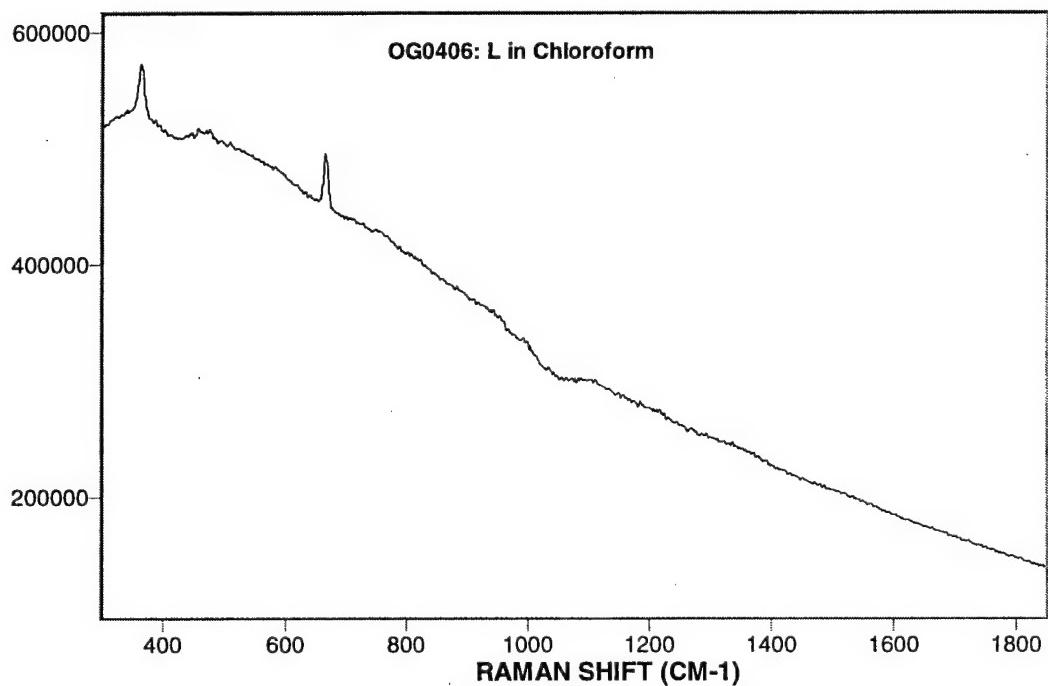


Figure C- 12: CAIS item OG0406 (lewisite in chloroform)

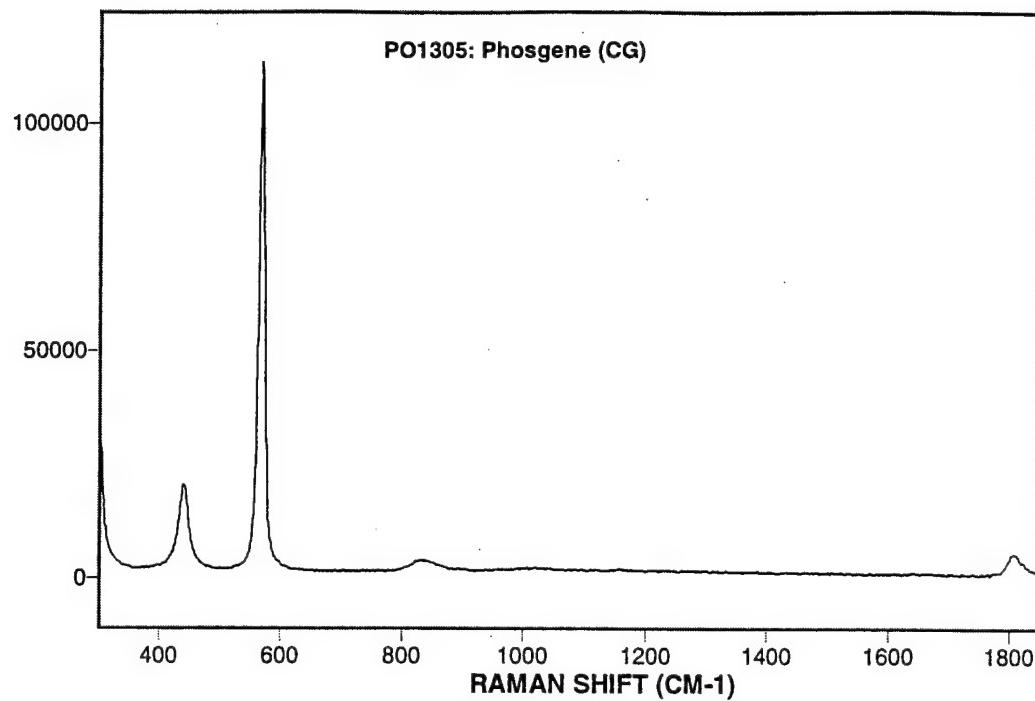


Figure C- 13: CAIS item PO1305 (phosgene)

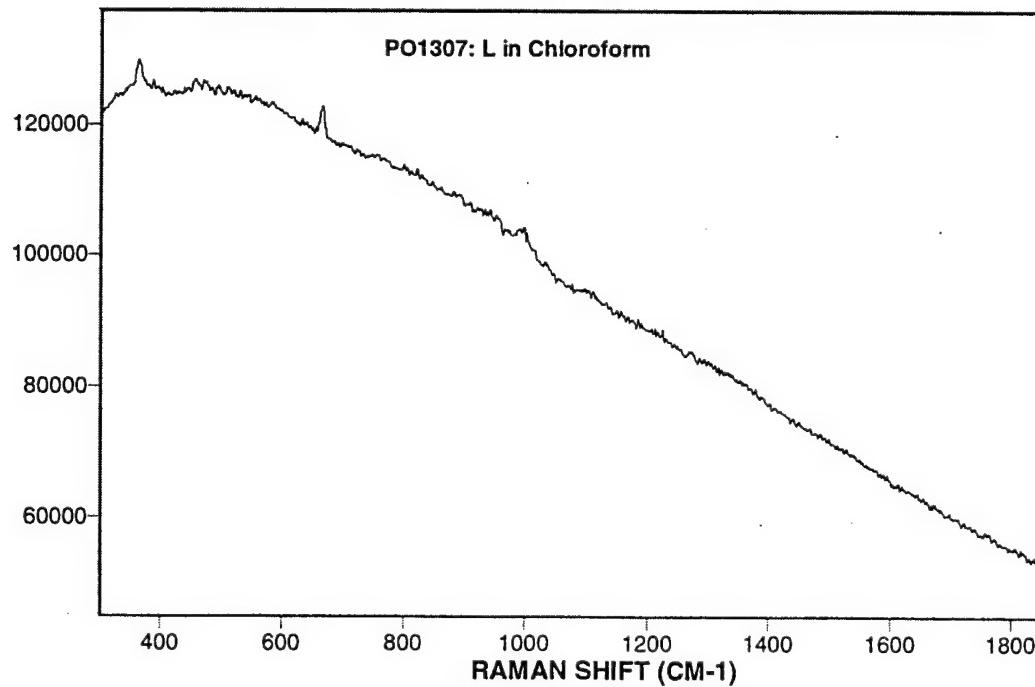


Figure C- 14: CAIS item PO1307 (lewisite in chloroform)

APPENDIX D: Spectra Obtained with the RS2000 Raman System.

FIGURES

D- 1: Adamsite (DM)	52
D- 2: Chloroacetophenone (CN)	52
D- 3: 50% Chloropicrin in Chloroform.....	53
D- 4: Mustard (HD).....	53
D- 5: 5% HD in Chloroform	54
D- 6: Cyanogen Chloride (CK)	54
D- 7: 5% L in Chloroform.....	55
D- 8: Phosgene	55
D- 9: CAIS item OG0101 (chloropicrin in chloroform)	56
D- 10: CAIS item FTOD023 (3.39% L in chloroform)	56
D- 11: CAIS item OG0206 (mustard in chloroform)	57

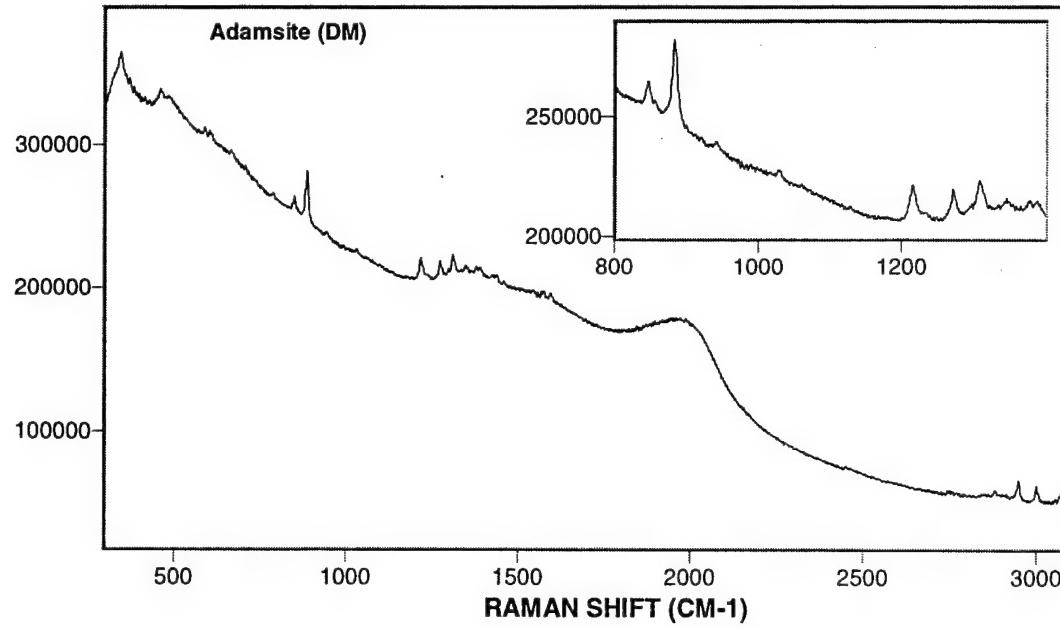


Figure D- 1: Adamsite (DM)

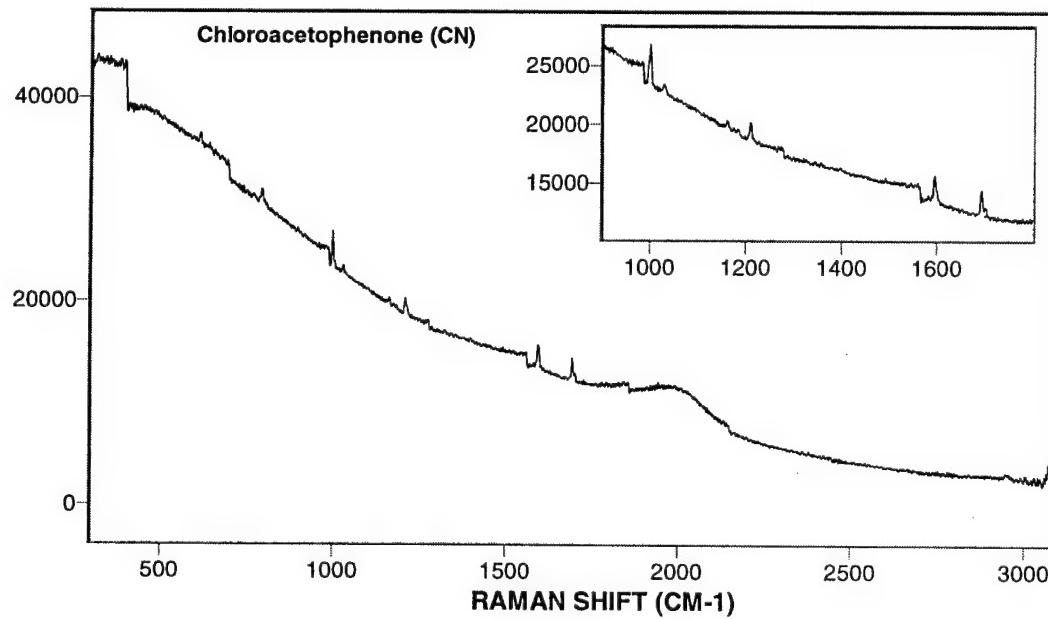


Figure D- 2: Chloroacetophenone (CN)

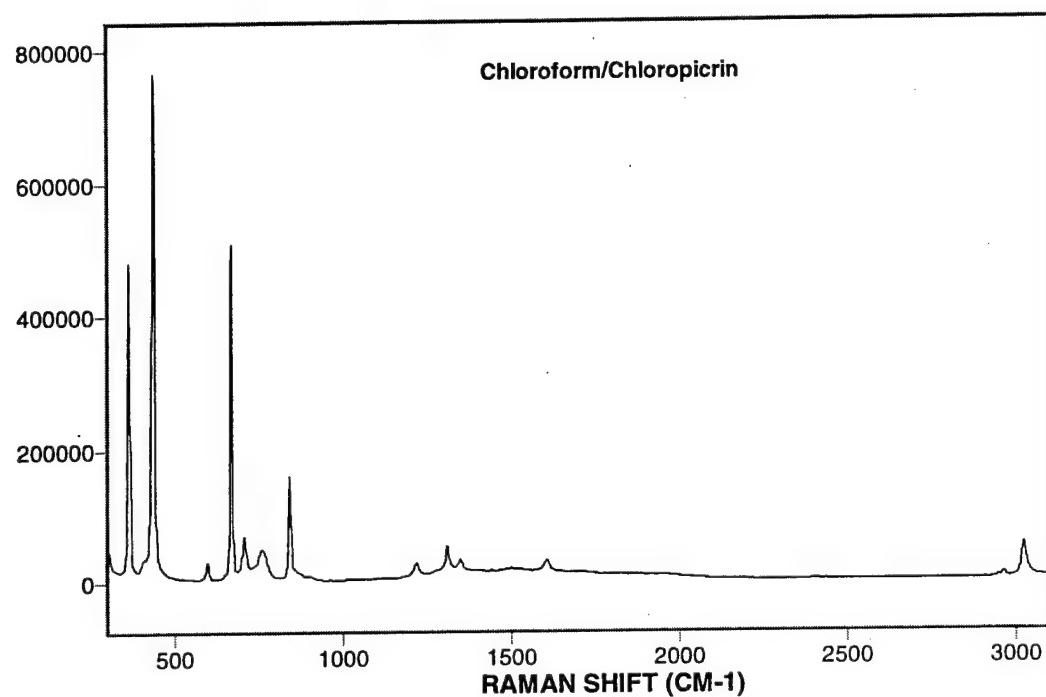


Figure D- 3: 50% Chloropicrin in Chloroform

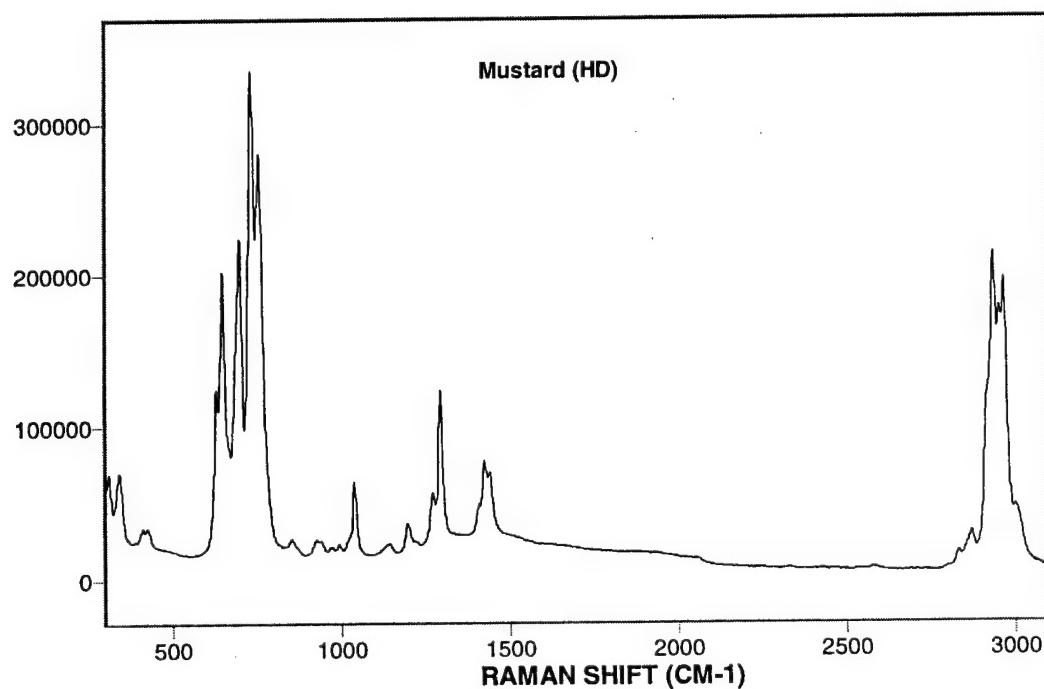


Figure D- 4: Mustard (HD)

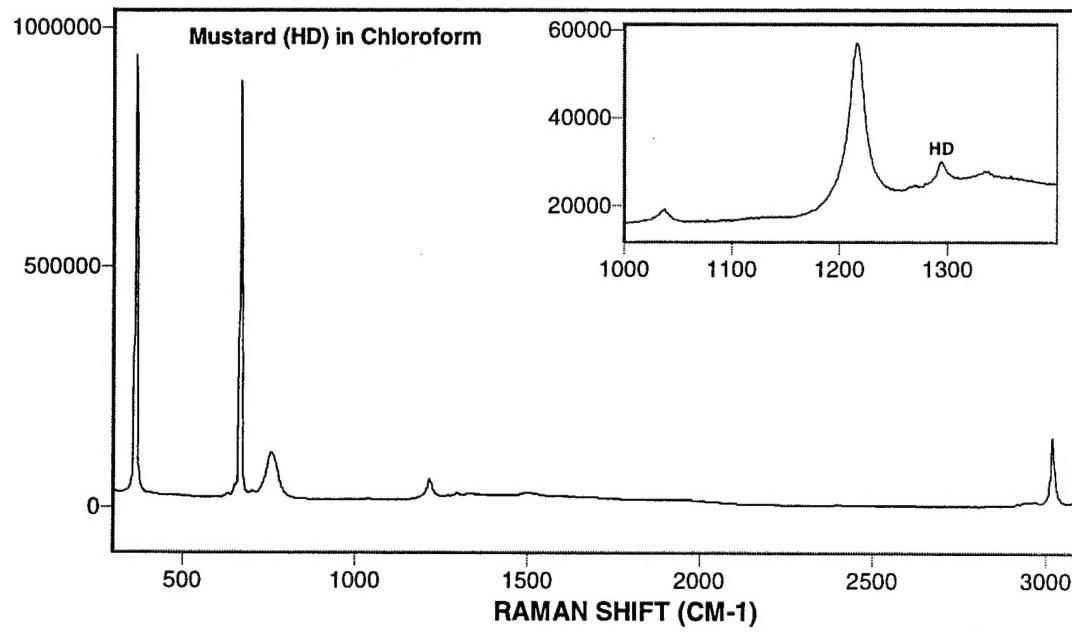


Figure D- 5: 5% HD in Chloroform

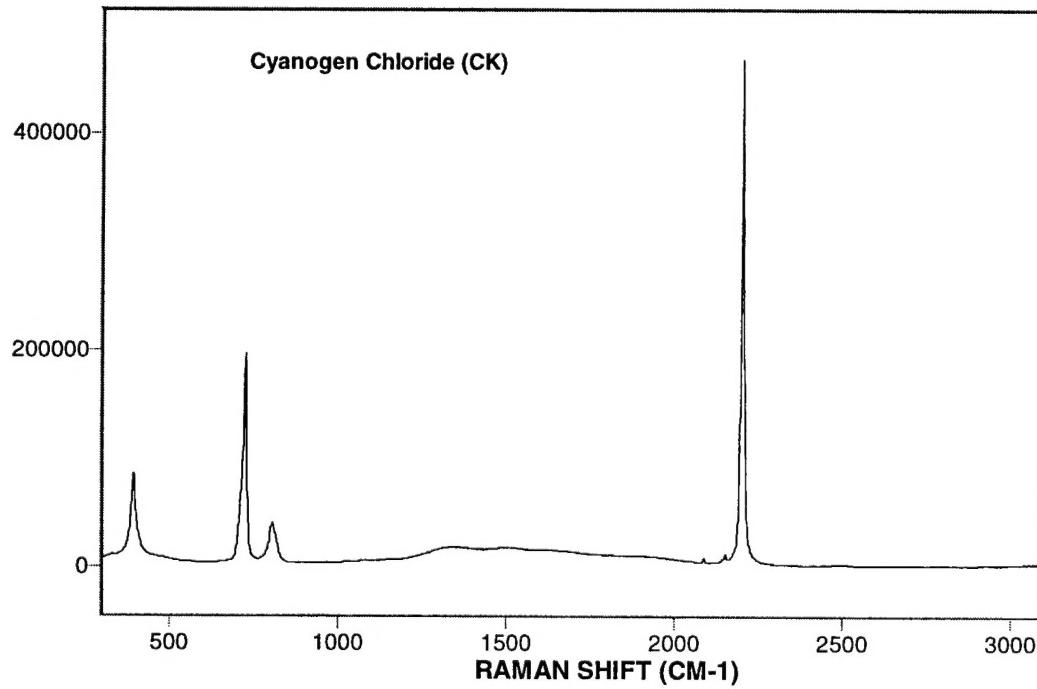


Figure D- 6: Cyanogen Chloride (CK)

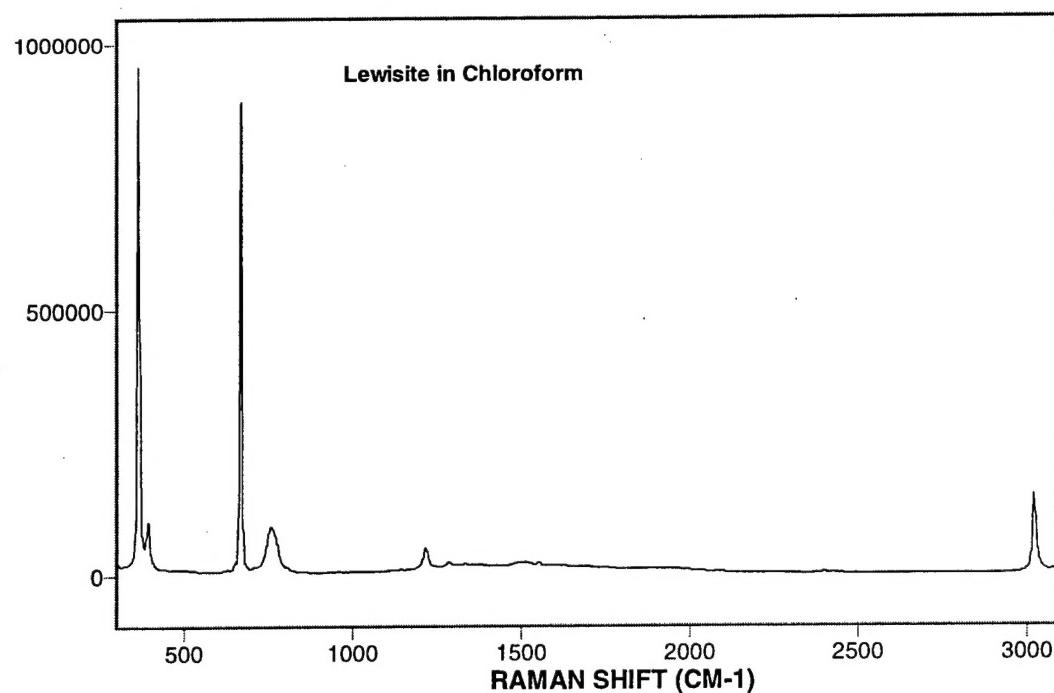


Figure D- 7: 5% L in Chloroform

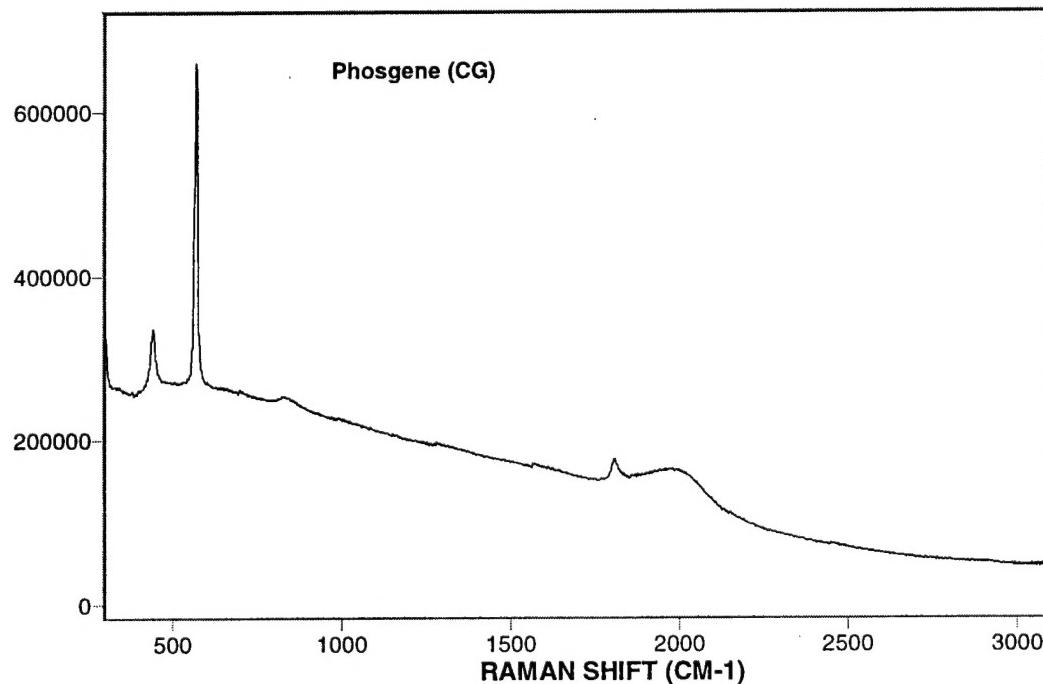


Figure D- 8: Phosgene

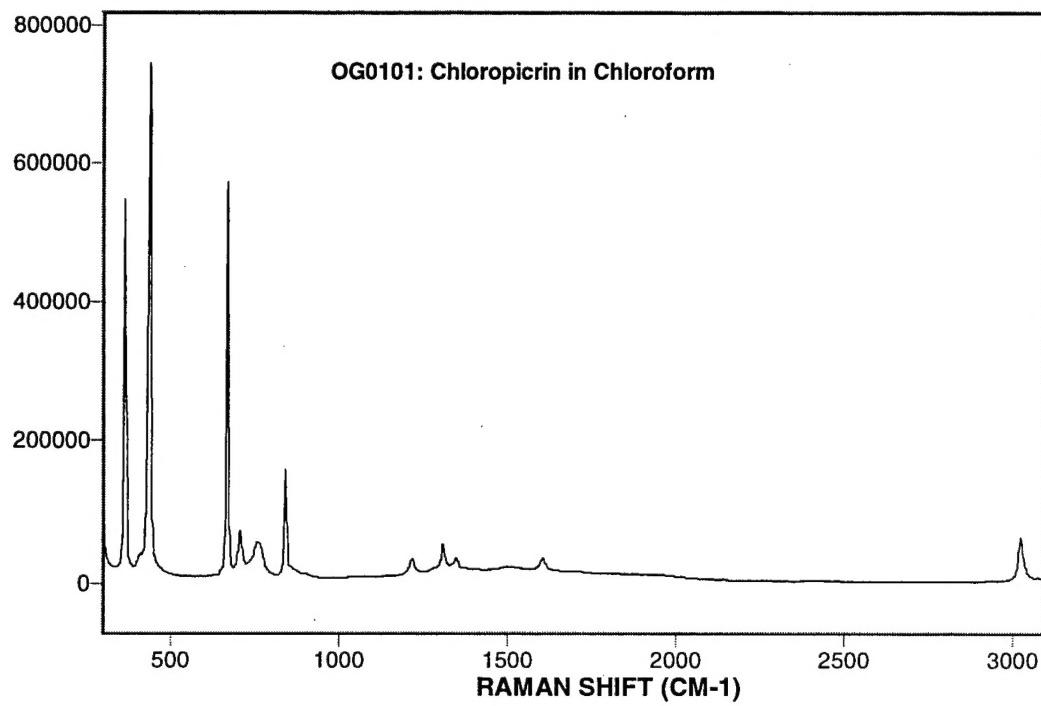


Figure D- 9: CAIS item OG0101 (chloropicrin in chloroform)

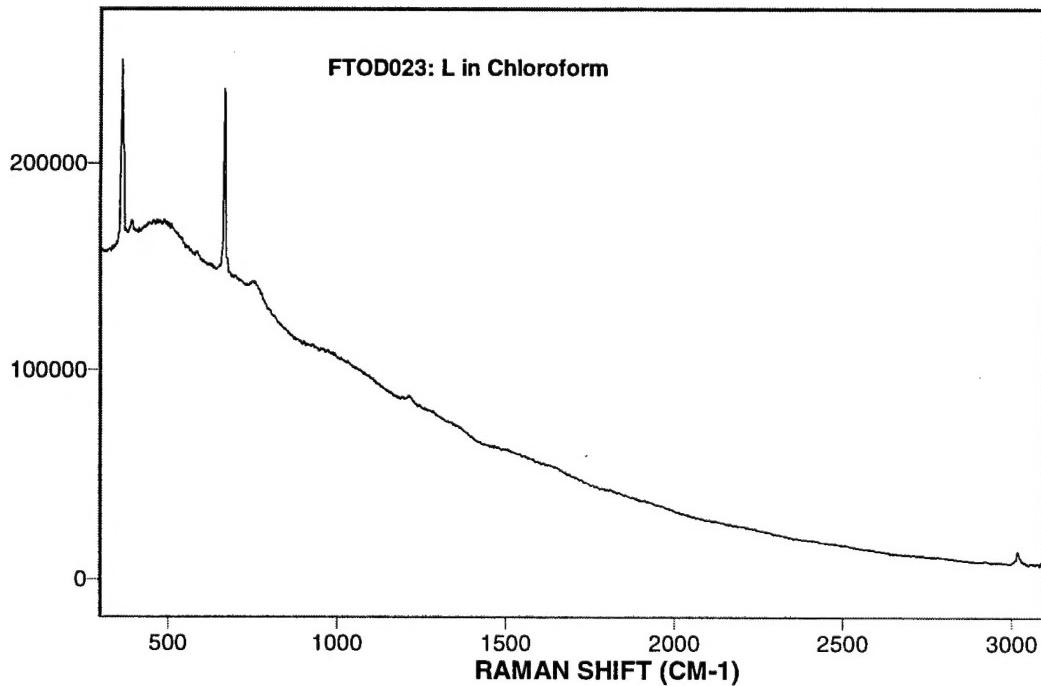


Figure D- 10: CAIS item FTOD023 (3.39% L in chloroform)

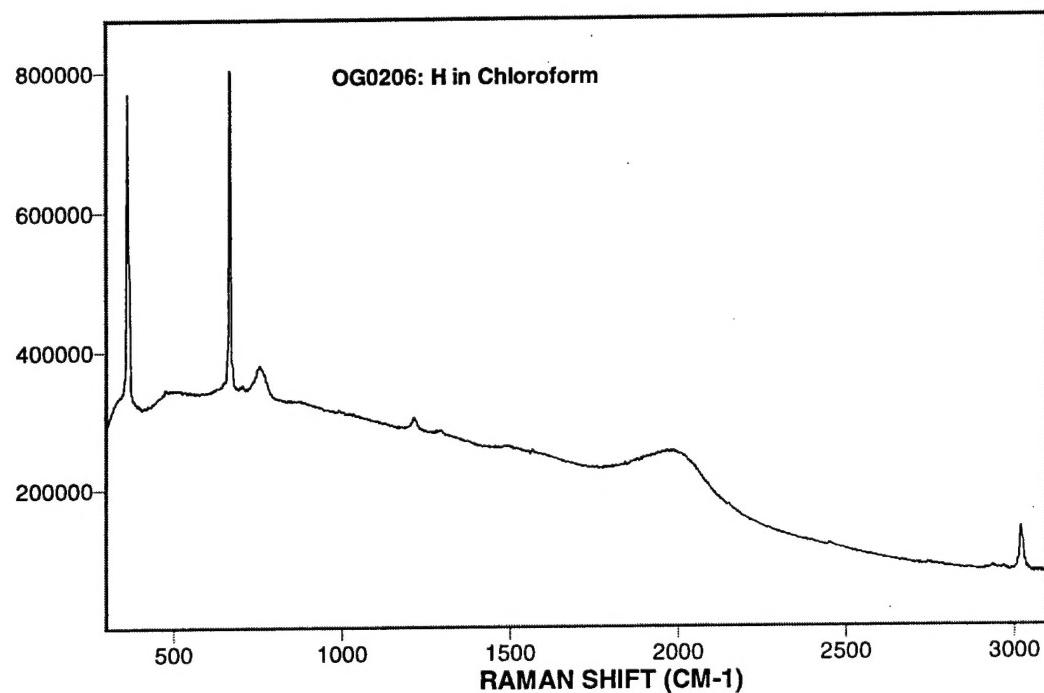


Figure D- 11: CAIS item OG0206 (mustard in chloroform)